THE THERMODYNAMIC PRESSURE OF A DILUTE FERMI GAS

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Abstract

We consider a gas of fermions with non-zero spin at temperature T and chemical potential μ. We show that if the range of the interparticle interaction is small compared to the mean particle distance, the thermodynamic pressure differs to leading order from the corresponding expression for non-interacting particles by a term proportional to the scattering length of the interparticle interaction. This is true for any repulsive interaction, including hard cores. The result is uniform in the temperature as long as T is of the same order as the Fermi temperature, or smaller.

1 Introduction and Main Results

The physics of dilute gases at low temperature has received a lot of interest in the last couple of years, due to the recent experimental advances in studying these systems. Despite tremendous interest in the problem, rigorous results starting from first principles remain sparse, and often one has to rely on uncontrolled approximations to obtain quantitative information. This is true especially for *dilute* systems, where the interparticle interaction can not easily be taken into account using perturbation theory. Here, dilute

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refers to the case when the range of the interparticle interaction is small compared with the mean particle distance.

The first, although admittedly not the most interesting, question to ask is for the ground state energy of the system. In [7], Lieb and Yngvason devised a method for proving the relevant expression for dilute Bose gases. In this case, the energy per unit volume at density ϱ is given by $4\pi a\varrho^2$, where a is the (s-wave) scattering length of the interaction potential, and $a^3\varrho \ll 1$, i.e., the system is dilute. (Units are chosen such that $\hbar = 1$ and $2m = 1$, where m denotes the mass of the particles.) The corresponding expression for a two-dimensional Bose gas was later proved in [8].

Recently, it was possible to extend these methods and prove the corresponding result for fermions [4]. That is, the ground state energy density of a dilute gas of spin q fermions is given by

$$\frac{3}{5}\left(\frac{6\pi^2}{q}\right)^{2/3}\varrho^{5/3} + 4\pi a\varrho^2\left(1 - q^{-1}\right) + \text{ higher order in } (a^3\varrho)\,. \tag{1.1}$$

As before, a denotes the scattering length. The factor $(1 - q^{-1})$ in the interaction energy results from the fact that only particles with different spin can exhibit s-wave scattering. The contribution from the interaction between particles of the same spin is of higher order in ϱ.

In this paper, we prove the analogue of (1.1) at positive temperature. Our main result is Theorem 1. We work in the grand canonical ensemble, and consider the pressure of the gas at given temperature T and chemical potential μ. We will show that, for dilute gases, the effect of the particle interaction results in a contribution $-4\pi a\varrho^2(1-q^{-1})$ to the pressure, where ϱ is now the average density. This result holds for any temperature, as long as T is not much bigger than the Fermi temperature (for the non-interacting gas), given by $T_{\rm F} = (6\pi^2/q)^{2/3}\varrho^{2/3}$ (in units where $k_{\rm B} = 1$). The rational behind this formula is the following: for dilute gases, the effect of the interaction reduces to two-particle s-wave scattering, which can take place only between particles of unequal spin. This is just like in the zero-temperature (ground state) case. The effect of the temperature on this scattering process is negligible, since for $T \lesssim T_{\rm F}$, the thermal wave length is of the same order (or greater) than the mean-particle distance. The aim of this paper is to make this intuition precise.

We will now describe the system in detail. For simplicity, we consider here only the case $q = 2$, i.e., the spin 1/2 case. The extension to $q > 2$ is straightforward. The Hilbert space under consideration is given by the

fermionic Fock space for spin 1/2 particles, $\mathcal{F} = \mathcal{F}_{\rm F}(L^2(\Lambda_L;\mathbb{C}^2))$. Here, Λ_L denotes a cube of side length L. The Hamiltonian is the direct sum $H = \bigoplus_{N=0}^{\infty} H_N$, with $H_0 = 0$, $H_1 = -\Delta$, and

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1\leq i<j\leq N} v(x_i - x_j) \tag{1.2}$$

for $N \geq 2$. Here, Δ denotes the Laplacian with Dirichlet boundary conditions on Λ_L. Units are chosen such that $\hbar = 1$ and $2m = 1$, where m denotes the mass of the particles. We note that both H and $\mathcal{F}$ depend on L, of course, but we suppress this dependence in our notation.

The pair potential v is assumed to be positive, radial, and of finite range R_0. It then has a finite and positive scattering length a. The scattering length may be defined as follows: if φ is the unique solution of the zero-energy scattering equation

$$-\Delta\varphi + \tfrac{1}{2}v\varphi = 0 \tag{1.3}$$

subject to the boundary condition $\lim_{|x|\to\infty}\varphi(x) = 1$, then a is given by $a = \lim_{|x|\to\infty}|x|(1-\varphi(x))$ (see Appendix A in [8] for details). Note that we do not assume v to be integrable, our results also apply to the case of a hard core. Note also that for a pure hard-core interaction, the scattering length is equal to the range.

Our main result concerns the pressure of the system at some given inverse temperature $\beta = 1/(k_{\rm B}T)$ and chemical potential μ. It is given by

$$P(\beta,\mu) = \lim_{L\to\infty}\frac{1}{L^3\beta}\ln \mathrm{Tr}_{\mathcal{F}}\, \exp\big(-\beta(H-\mu\hat{N})\big)\,. \tag{1.4}$$

Here, $\hat{N}$ denotes the number operator. It is well known that for systems with short range interactions the limit in (1.4) exists and is independent of boundary conditions [9, 10].

We are interested in $P(\beta,\mu)$ for low density, ϱ, which is given by $\varrho = \partial P/\partial\mu$, assuming the derivative exists. (Note that $P(\beta,\mu)$ is convex in μ and therefore the derivative exists almost everywhere. In particular, the right and left derivatives exist.) With *low density* we mean that the dimensionless quantity $a^3\varrho$ is small, i.e., that the gas is *dilute*. Note that there are two dimensionless quantities in this problem: $a^3\varrho$, measuring the diluteness, and the fugacity $z = e^{\beta\mu}$. Small z corresponds to the (high temperature) limit of a classical gas, whereas for large z the system approaches its ground state. Since we are interested in the quantum aspects of the system, we will

consider the case when $1/z$ is bounded. Another way of saying the same thing is that there are three length scales in the problem: the scattering length a, the mean particle distance $\varrho^{-1/3}$, and the thermal wavelength $\beta^{1/2}$. We are interested in the regime where $a \ll \varrho^{-1/3} \lesssim \beta^{1/2}$, i.e., where a is much smaller than $\varrho^{-1/3}$ and $\varrho^{-1/3}$ is comparable with, or much smaller than, $\beta^{1/2}$.

Let $P_0(\beta, \mu)$ and $\varrho_0(\beta, \mu)$ be the pressure and density of a non-interacting gas of spin 1/2 fermions. They are given by

$$P_0(\beta, \mu) = \frac{2}{\beta}(2\pi)^{-3} \int_{\mathbb{R}^3} dp \, \ln\left(1 + z \exp(-\beta p^2)\right) \tag{1.5}$$

and

$$\varrho_0(\beta, \mu) = \frac{\partial P_0(\beta, \mu)}{\partial \mu} = 2(2\pi)^{-3} \int_{\mathbb{R}^3} dp \, \frac{1}{1 + z^{-1} \exp(\beta p^2)}, \tag{1.6}$$

respectively. The factor 2 in front of the integrals takes the number of spin states into account.

Our main result is the following.

THEOREM 1. *Let $\varrho_0 \equiv \varrho_0(\beta, \mu)$ and let $z = e^{\beta\mu}$. For any $\alpha < 1/33$ there exists a function $C_\alpha(z)$, uniformly bounded in z for bounded $1/z$, such that*

$$\left| P(\beta, \mu) - P_0(\beta, \mu) + 2\pi a \varrho_0(\beta, \mu)^2 \right| \leq C_\alpha(z) a \varrho_0^2 \left(a \varrho_0^{1/3}\right)^\alpha . \tag{1.7}$$

We remark that the non-uniformity of our bound for small z is not an artifact of our method of proof. In the limit $z \to 0$ one obtains a classical gas where $2\pi a \varrho_0^2$ certainly does *not* give the correct contribution of the interaction at low density. In particular, this term depends on Planck's constant (which equals 1 in our units).

Our proof below gives explicit bounds on the $C_\alpha(z)$ appearing in the statement of the theorem. Since the exponent α in the error term on the right side of (1.7) is far from optimal, however, we did not make the effort of writing down these bounds explicitly. Moreover, $C_\alpha(z)$ depends on the interaction potential v only through its range or, more precisely, through the dimensionless ratio R_0/a. Also this dependence could in principle be given explicitly.

We note that $\varrho_0(\beta, \mu)$ can be replaced by the true density (of the interacting gas) in Eq. (1.7). In fact, we have the following corollary of Theorem 1.

COROLLARY 1. *Let $\varrho_\pm(\beta, \mu) = \partial P(\beta, \mu)/\partial \mu^\pm$ denote the right and left derivatives of $P(\beta, \mu)$, respectively. For any $\alpha < 1/33$ there exists a function*

$\widehat{C}_\alpha(z)$*, uniformly bounded in* z *for bounded* $1/z$*, such that*

$$\frac{|\varrho_\pm(\beta,\mu) - \varrho_0(\beta,\mu)|}{\varrho_0(\beta,\mu)} \leq \widehat{C}_\alpha(z)\big(a\varrho_0^{1/3}\big)^{(1+\alpha)/2} . \tag{1.8}$$

The proof of Theorem 1 will actually not only show that the density of the interacting and non-interacting system are close, as claimed in (1.8), but also the reduced one-particle density matrices (cf. Eq. (4.61)). It is to expect that $\varrho_\pm(\beta,\mu) = \varrho_0(\beta,\mu) - 2\pi a \partial\varrho_0(\beta,\mu)/\partial\mu +$ higher order terms in $a^3\varrho_0$, but we do not have a proof of this claim. Nevertheless, we note that Theorem 1 implies a similar statement for other thermodynamic potentials. We state the following corollary for the Helmholtz free energy, but an analogous result holds for other thermodynamic potentials as well.

COROLLARY 2. *For* $\varrho > 0$*, let* $f(\beta,\varrho) = \sup_\mu[\mu\varrho - P(\beta,\mu)]$ *denote the free energy density, and* $f_0(\beta,\varrho)$ *the corresponding quantity for the non-interacting system. For any* $\alpha < 1/33$ *there exists a function* $\widetilde{C}_\alpha(x)$*, uniformly bounded in* x *for bounded* $1/x$*, such that*

$$\big|f(\beta,\varrho) - f_0(\beta,\varrho) - 2\pi a\varrho^2\big| \leq \widetilde{C}_\alpha\big(\beta\varrho^{2/3}\big)a\varrho^2\big(a\varrho^{1/3}\big)^\alpha . \tag{1.9}$$

Theorem 1 (and Corollaries 1 and 2) can be extended in several ways, as will be explained now. For simplicity, we omit the proof of these assertions here. They can be proved by only small modifications of the proof of Theorem 1 given below, which is already quite lengthy itself.

- *Polarized gas:* A term $mS^3_{\rm tot}$ can be added to the Hamiltonian, where $S^3_{\rm tot}$ denotes the 3-component of the total spin of the particles, and m is a coupling parameter proportional to the magnetic field. This has the effect of adding a 'spin-dependent' chemical potential. Theorem 1 also holds in this case (with P and P_0 depending on m, of course), if $2\pi a\varrho^2$ is replaced by $8\pi a\varrho_\downarrow\varrho_\uparrow$. Here, $\varrho_\downarrow$ and $\varrho_\uparrow$ denote the density of spin-up and spin-down particles, respectively. They are given by derivatives of the pressure as $\frac{1}{2}\partial P/\partial\mu \pm \partial P/\partial m$.

- *Higher spin:* The case of higher spin can be treated in the same way. If q denotes the number of spin states, then the leading order contribution of the interaction energy per unit volume for a dilute gas is $4\pi a(1-q^{-1})\varrho^2$, which reduces to (1.7) in the case $q = 2$. Also the polarized gas can be studied for spin higher then $1/2$.

- *Infinite range potentials:* As already mentioned, the error term on the right side of (1.7) depends on the interaction potential only through the ratio of its range to its scattering length, R_0/a. By cutting off the potential v in an appropriate (ϱ-dependent) way, it is therefore possible to extend Theorem 1 to infinite range potentials (with finite scattering length), with possibly a worse error term than the one given in (1.7). (Compare with the corresponding discussion for the Bose gas in the appendices of [5] and [8].)

- *The two-dimensional gas:* A corresponding result can also be derived for a Fermi gas in two dimensions. The leading contribution of the interaction energy for a dilute gas is then $2\pi\varrho^2/|\ln a^2\varrho|$ per unit volume. This was shown in [4] for the ground state, i.e., at zero temperature, and the methods developed in this paper can be used to obtain this result also at positive temperature.

Before giving the full proof of Theorem 1, we start with a short outline to guide the reader. In the next Section 2, we state some preliminaries that will be useful for our proofs. We introduce the pressure functional which defines a variational principle for the pressure. We also state some useful properties of the non-interacting system. Sections 3 and 4 contain the proof of Theorem 1. This proof is divided into two parts, the lower and upper bounds to the pressure. Finally, in Section 5, we give the proof of Corollaries 1 and 2.

For the lower bound to the pressure, given in Section 3, it is necessary to construct an appropriate trial density matrix for the pressure functional. As in the zero temperature calculation in [4], we find it necessary to choose a trial density matrix that confines particles into small boxes in order to control the average particle number in each box. The construction in each small box is done in Subsect. 3.2. We then proceed with the calculation of the variational pressure in Subsect. 3.3. We use similar methods as in [4] to estimate the energy of the state. In addition, it is necessary to estimate its entropy, which is done with the aid of Lemma 2. The price one has to pay for using the box method are finite size corrections, which are estimated in Subsect. 3.4. The final result is then stated in Subsect. 3.5.

The upper bound to the pressure, given in Section 4, has two main ingredients. First, an operator inequality proved in [4, Lemma 4], which allows for the replacement of the interaction potential v by a "soft" potential U, at the expense of the high-momentum part of the kinetic energy. See Subsect. 4.1. Secondly, an improved version of subadditivity of entropy in

Subsect. 4.2, which was recently derived in [3]. As shown in Subsect. 4.3, this estimate allows to prove that the reduced one-particle density matrix of the spin-up particles, for *fixed* positions of the spin-down particles, is close to the Fermi-Dirac distribution for non-interacting particles. This property of the reduced one-particle density matrix is then used to show, in Subsect. 4.4, that first order perturbation theory with the soft potential U gives the correct answer for dilute gases.

2 Preliminaries

Since the Hamiltonian H does not depend on the spin variables and, in particular, commutes with the operators counting the number of spin-up and spin-down particles, the problem can be reformulated in terms of two species of spinless fermions. More precisely, $\mathcal{F} \cong \mathcal{F}_{\mathrm{F}}(\mathcal{H}_1) \otimes \mathcal{F}_{\mathrm{F}}(\mathcal{H}_1) \equiv \mathcal{F}_\uparrow \otimes \mathcal{F}_\downarrow$, where $\mathcal{H}_1 = L^2(\Lambda_L; \mathbb{C})$ denotes the one-particle space for *spinless* particles. We label particle coordinates in the first factor by $x^\uparrow$ and in the second by $x^\downarrow$. The Hamiltonian in this representation can then be written as $H = \bigoplus_{N,M=0}^{\infty} H_{N,M}$, with

$$\begin{aligned} H_{N,M} &= -\sum_{i=1}^{N} \Delta_i^\uparrow - \sum_{k=1}^{M} \Delta_k^\downarrow + \sum_{i=1}^{N} \sum_{k=1}^{M} v(x_i^\uparrow - x_k^\downarrow) \\ &\quad + \sum_{1 \le i < j \le N} v(x_i^\uparrow - x_j^\uparrow) + \sum_{1 \le k < l \le M} v(x_k^\downarrow - x_l^\downarrow) \,. \end{aligned} \tag{2.1}$$

The first two terms are simply the kinetic energies of the spin-up and spin-down particles, and the interaction potential is divided into three parts, corresponding to interaction between particles of the same and of different spin, respectively. In a sector of fixed particle numbers N and M, we denote the particle coordinates collectively by $X^\uparrow = (x_1^\uparrow, \ldots, x_N^\uparrow)$ and $X^\downarrow = (x_1^\downarrow, \ldots, x_M^\downarrow)$.

2.1 The Pressure Functional

The pressure (1.4) can be computed via a variational principle. For Γ a density matrix, i.e., a positive trace class operator on $\mathcal{F}$ with $\mathrm{Tr}_{\mathcal{F}}\, \Gamma = 1$, we define the pressure functional $\mathcal{P}^L[\Gamma]$ by

$$-L^3\, \mathcal{P}^L[\Gamma] = \mathrm{Tr}_{\mathcal{F}} \left[(H - \mu \hat{N}) \Gamma \right] - \frac{1}{\beta} S[\Gamma] \,, \tag{2.2}$$

where $S[\Gamma] = -\mathrm{Tr}_{\mathcal{F}}\,(\Gamma \ln \Gamma)$ denotes the (von Neumann) entropy. (The expression (2.2) is well defined if the eigenfunctions of Γ are in the quadratic form domain of H and $\hat{N}$. Otherwise, we can take it to be $+\infty$.) Let $P^L(\beta, \mu)$ denote the maximum of $\mathcal{P}^L[\Gamma]$ over all density matrices. The maximum is uniquely attained by the grand-canonical Gibbs density matrix, given by $\exp(-\beta(H - \mu\hat{N}))/\mathrm{Tr}_{\mathcal{F}} \exp(-\beta(H - \mu\hat{N}))$. Hence the pressure $P^L(\beta, \mu)$ is given by $P^L(\beta, \mu) = L^{-3}\beta^{-1} \ln \mathrm{Tr}_{\mathcal{F}} \exp\left(-\beta(H - \mu\hat{N})\right)$, and $P(\beta, \mu) = \lim_{L\to\infty} P^L(\beta, \mu)$.

At zero temperature, i.e., when $\beta = \infty$, this variational principle reduces to the usual variational principle for the ground state energy. Note, however, that at positive temperature the functional (2.2) is not linear in the density matrix.

2.2 The Ideal Fermi Gas

For later use, we also define the pressure functional for the noninteracting gas, $\mathcal{P}_0^L[\Gamma]$. It is defined in the same way as $\mathcal{P}^L[\Gamma]$ above, with H replaced by the non-interacting Hamiltonian $H^{(0)} = \bigoplus_{N,M=0}^{\infty} H_{N,M}^{(0)}$, where $H_{N,M}^{(0)}$ is given as in (2.1) but with $v = 0$. We denote the (finite volume) pressure for the non-interacting gas by $P_0^L(\beta, \mu)$. It is given by

$$P_0^L(\beta, \mu) = \frac{2}{\beta} \frac{1}{L^3} \mathrm{Tr}_{\mathcal{H}_1} \ln\left(1 + z \exp(\beta\Delta)\right), \tag{2.3}$$

which reduces to (1.5) in the thermodynamic limit. We note that this expression can also be obtained from a variational principle for the reduced one-particle density matrix (see, e.g., [12]). Namely,

$$-\tfrac{1}{2} L^3 P_0^L(\beta, \mu) = \inf_{\gamma} \left[\mathrm{Tr}_{\mathcal{H}_1}(-\Delta - \mu)\gamma - \frac{1}{\beta}\widetilde{S}[\gamma] \right], \tag{2.4}$$

where the infimum is over all positive trace class operators γ on $\mathcal{H}_1$ with $0 \leq \gamma \leq 1$, and $\widetilde{S}[\gamma]$ is given by

$$\widetilde{S}[\gamma] = \mathrm{Tr}_{\mathcal{H}_1}\left[-\gamma \ln \gamma - (1 - \gamma)\ln(1 - \gamma)\right]. \tag{2.5}$$

The reason for the factor 1/2 in front of P_0^L are the 2 different spin states, which we have not accounted for in the functional. The infimum in (2.4) is uniquely attained at $\gamma_0 = (1 + z^{-1}e^{-\beta\Delta})^{-1}$.

3 Lower Bound to the Pressure

We start the proof of Theorem 1 by deriving a lower bound to the pressure. Since $P(\beta,\mu)$ is determined by maximizing the pressure functional, a lower bound can be derived using an appropriate trial density matrix in the pressure functional (2.2).

3.1 The Box Method

It will be convenient to divide space into small boxes of side length ℓ and confine the particles to these boxes. By choosing ℓ appropriately, we can then control the average particle number in every box. Moreover, if we keep these boxes separated by a distance R_0, there is no interaction between particles in different boxes.

More precisely, pick an integer I and divide the interval $[0,L]$ into I intervals of equal length. We choose I such that $\ell \equiv L/I - R_0 > 0$. From the variational principle defined by (2.2) we can infer that

$$L^3 P^L(\beta,\mu) \geq I^3 \ell^3 P^\ell(\beta,\mu)\,, \tag{3.1}$$

where the factor I^3 is the number of boxes. Dividing (3.1) by L^3 and letting $L\to\infty$ and $I\to\infty$ in such a way that L/I converges to some number greater than R_0, we see that

$$P(\beta,\mu) \geq \frac{1}{(1+R_0/\ell)^3} P^\ell(\beta,\mu) \tag{3.2}$$

for any $\ell > 0$.

3.2 Construction of the Trial Density Matrix

We now construct a trial density matrix for $\mathcal{P}^\ell[\Gamma]$. For fixed β and μ, let $\varrho_0 = \varrho_0(\beta,\mu)$, and let $K>0$. Let Q be the projector onto the subspace of $\mathcal{H}_1 = L^2(\Lambda_\ell;\mathbb{C})$ where $-\Delta \leq K\varrho_0^{2/3}$, i.e., $Q = \theta(K\varrho_0^{2/3} + \Delta)$. Here, θ denotes the Heaviside step function, given by

$$\theta(t) = \begin{cases} 0 & \text{for } t<0 \\ 1 & \text{for } t\geq 0\,. \end{cases} \tag{3.3}$$

On $\mathcal{F}_Q \equiv \mathcal{F}(Q\mathcal{H}_1)\otimes\mathcal{F}(Q\mathcal{H}_1)$, let H_Q denote the second quantization of $-\Delta Q$, and let Γ_Q be the corresponding grand canonical Gibbs density matrix, defined as $\Gamma_Q = \exp(-\beta(H_Q - \mu\hat{N}))/\mathrm{Tr}_{\mathcal{F}_Q}\exp(-\beta(H_Q-\mu\hat{N}))$. We use

the same symbol for the density matrix on $\mathcal{F}$, being Γ_Q on the subspace $\mathcal{F}_Q$ and 0 on the orthogonal complement. Let $\varrho_Q = \ell^{-3}\mathrm{Tr}_{\mathcal{F}}\hat{N}\Gamma_Q$ be the average density of Γ_Q. By explicit computation,

$$\varrho_Q = \frac{2}{\ell^3}\mathrm{Tr}_{\mathcal{H}_1}\, Q\frac{1}{1+\exp(\beta(-\Delta-\mu))}\,. \tag{3.4}$$

We can decompose Γ_Q as

$$\Gamma_Q = \sum_\alpha \lambda_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|\,, \tag{3.5}$$

with $\lambda_\alpha \geq 0$, $\sum_\alpha \lambda_\alpha = 1$, and $\{\psi_\alpha\}$ an orthonormal set in $\mathcal{F}_Q$. Moreover, we can always choose the ψ_α to be products of Slater determinants of N_α $\uparrow$-particles and M_α $\downarrow$-particles, respectively, for some $N_\alpha, M_\alpha \in \mathbb{N}$. Given such a ψ_α, we define

$$\phi_\alpha = \frac{F^{N_\alpha,M_\alpha}\psi_\alpha}{\|F^{N_\alpha,M_\alpha}\psi_\alpha\|}\,, \tag{3.6}$$

with $F^{N,M}$ given as follows. Pick some $s > 2R_0$ and let $g : \mathbb{R}^3 \mapsto \mathbb{R}$ be function with $0 \leq g \leq 1$, having the property that $g(x) = 0$ for $|x| \leq s$ and $g(x) = 1$ for $|x| \geq 2s$. We may also assume that $|\nabla g| \leq \mathrm{const.}\, s^{-1}$ for some constant independent of s. Moreover, for some $\frac{1}{2}s \geq R > R_0$, let $f : \mathbb{R}^3 \mapsto \mathbb{R}$ be given by $f(x) = \varphi(x)/(1-a/R)$ for $|x| \leq R$ and 1 otherwise. Here, φ denotes the solution to the zero-energy scattering equation (1.3). Note that f is a continuous function, since $\varphi(x) = 1 - a/|x|$ for $|x| \geq R_0$. We define

$$F^{N,M}(X^\uparrow, X^\downarrow) = \prod_{1\leq i<j\leq N} g(x_i^\uparrow - x_j^\uparrow) \prod_{1\leq k<l\leq M} g(x_k^\downarrow - x_l^\downarrow) \prod_{i=1}^{N}\prod_{k=1}^{M} f(x_i^\uparrow - x_k^\downarrow)\,. \tag{3.7}$$

As a trial density matrix for $\mathcal{P}^\ell[\Gamma]$ we choose

$$\Gamma = \sum_\alpha \lambda_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|\,, \tag{3.8}$$

with ϕ_α defined by (3.6) and (3.7). Note that the ϕ_α are not orthogonal, but they are normalized, and hence $\mathrm{Tr}_{\mathcal{F}}\,\Gamma = 1$.

3.3 Calculation of the Variational Pressure

We now derive a lower bound on the variational pressure $\mathcal{P}^\ell[\Gamma]$, with Γ given in (3.8). We start with the expectation value of the energy,

$$\mathrm{Tr}_{\mathcal{F}}\, H\Gamma = \sum_\alpha \lambda_\alpha \langle\phi_\alpha|H_{N_\alpha,M_\alpha}|\phi_\alpha\rangle\,, \tag{3.9}$$

which we have to bound from above. This expression can be estimated using the same methods as in [4, Sect. IV]. More precisely, the calculation in [4] shows the following.

Lemma 1. *For $N, M \geq 0$, let D_1 and D_2 denote Slater determinants of N and M orthonormal eigenfunctions of the Dirichlet Laplacian on a cube of side length ℓ, respectively. Let k denote the maximal kinetic energy of these $N + M$ functions. Let $\psi(X^\uparrow, X^\downarrow) = D_1(X^\uparrow)D_2(X^\downarrow)F^{N,M}(X^\uparrow, X^\downarrow)$, with $F^{N,M}$ given in (3.7). Then, for some constant $c > 0$,*

$$\frac{\langle\psi|H_{N,M}|\psi\rangle}{\langle\psi|\psi\rangle} \leq \langle D_1 D_2|H^{(0)}_{N,M}|D_1 D_2\rangle + 8\pi a\frac{NM}{\ell^3}\left(1 + cN^{-1/3} + cM^{-1/3}\right)$$
$$+ca\frac{NM}{\ell^3}E\big(R, s, N+M, k, \ell\big) + c(N+M)^{7/3}\frac{s^{3/2}a^{1/2}}{\ell^4}\,, \tag{3.10}$$

where E is the function

$$E(R, s, n, k, \ell) = \frac{aR^2}{s^3} + s^2 k + \frac{a}{R} + n^{8/3}(s/\ell)^5\,. \tag{3.11}$$

This lemma was proved in [4] for the special case when D_1 and D_2 are Slater determinants of the lowest N and M eigenfunctions of the Dirichlet Laplacian, respectively (compare with [4, Eq. (46)]). The proof, however, goes through without change in the general case, the only difference being the maximal value of the kinetic energy, k, which enters the bound through the estimate in [4, Lemma 2]. More precisely, the value $n^{2/3}/\ell^2$ in [4, Lemma 2] has to be replaced by k in the general case considered here.

Note that the error term in Lemma 1 is not uniform in the particle number. For this reason, it is necessary to confine the particles into small boxes, as done here.

In the case of interest in (3.9), the number of particles is at most $N+M \leq 2\,\mathrm{Tr}_{\mathcal{H}_1} Q \leq c\ell^3 K^{3/2}\varrho_0$ for some constant $c > 0$, and the kinetic energy of each factor in the Slater determinants is at most $k \leq K\varrho_0^{2/3}$. Hence Lemma 1 implies the upper bound

$$\langle\phi_\alpha|H_{N_\alpha,M_\alpha}|\phi_\alpha\rangle \leq \langle\psi_\alpha|H^{(0)}_{N_\alpha,M_\alpha}|\psi_\alpha\rangle + 8\pi a\frac{N_\alpha M_\alpha}{\ell^3}\left(1 + cN_\alpha^{-1/3} + cM_\alpha^{-1/3}\right)$$
$$+ca\frac{N_\alpha M_\alpha}{\ell^3}E\big(R, s, K^{3/2}\varrho_0\ell^3, K\varrho_0^{2/3}, \ell\big)$$
$$+c(N_\alpha + M_\alpha)K^2\varrho_0^{4/3}s^{3/2}a^{1/2} \tag{3.12}$$

for some constant $c > 0$. We now insert this estimate into (3.9). We have

$$\sum_\alpha \lambda_\alpha N_\alpha M_\alpha = \mathrm{Tr}_{\mathcal{F}}\, \hat{N}^{\uparrow} \hat{N}^{\downarrow} \Gamma_Q = \left(\tfrac{1}{2}\ell^3 \varrho_Q\right)^2 , \tag{3.13}$$

where $\hat{N}^{\updownarrow}$ denotes the number operator on $\mathcal{F}_{\updownarrow}$. Moreover, using convexity of $x \mapsto x^{3/2}$, it follows from Jensen's inequality that

$$\sum_\alpha \lambda_\alpha N_\alpha^{2/3} M_\alpha \leq \left(\tfrac{1}{2}\ell^3 \varrho_Q\right)^{5/3} , \tag{3.14}$$

and likewise with N_α and M_α interchanged. Also $\sum_\alpha \lambda_\alpha (N_\alpha + M_\alpha) = \mathrm{Tr}_{\mathcal{F}} \hat{N} \Gamma_Q = \varrho_Q \ell^3$. Thus we obtain the upper bound

$$\begin{aligned} \mathrm{Tr}_{\mathcal{F}}\, H\Gamma \ \leq\ & \mathrm{Tr}_{\mathcal{F}}\, H^{(0)}\Gamma_Q + 2\pi a \varrho_Q^2 \ell^3 \Big(1 + c\Big[\ell^{-1}\varrho_Q^{-1/3} + K^2 \varrho_0^{4/3} \varrho_Q^{-1} s^{3/2} a^{-1/2} \\ & + E\big(R, s, K^{3/2}\varrho_0 \ell^3, K\varrho_0^{2/3}, \ell\big)\Big]\Big) \end{aligned} \tag{3.15}$$

for some constant $c > 0$.

The next step is to calculate the average particle number. By construction of Γ,

$$\mathrm{Tr}_{\mathcal{F}}\, \hat{N}\Gamma = \sum_\alpha \lambda_\alpha \langle \phi_\alpha | \hat{N} | \phi_\alpha \rangle = \sum_\alpha \lambda_\alpha \langle \psi_\alpha | \hat{N} | \psi_\alpha \rangle = \mathrm{Tr}_{\mathcal{F}}\, \hat{N}\Gamma_Q \,. \tag{3.16}$$

It remains to derive a lower bound on the entropy of Γ. For this purpose, we need the following Lemma.

Lemma 2. *Let Γ be a density matrix on some Hilbert space, with eigenvalues $\lambda_\alpha \geq 0$. For $\{P_\alpha\}$ (not necessarily orthogonal) one-dimensional projections, let $\widehat{\Gamma} = \sum_\alpha \lambda_\alpha P_\alpha$. Then*

$$S[\widehat{\Gamma}] \geq S[\Gamma] - \ln \left\| \textstyle\sum_\alpha P_\alpha \right\| . \tag{3.17}$$

Proof. Using twice concavity of the logarithm,

$$\begin{aligned} S[\widehat{\Gamma}] - S[\Gamma] &= -\sum_\alpha \lambda_\alpha \mathrm{Tr}\, P_\alpha \ln\left(\lambda_\alpha^{-1}\widehat{\Gamma}\right) \\ &\geq -\sum_\alpha \lambda_\alpha \ln \mathrm{Tr}\, P_\alpha \lambda_\alpha^{-1} \widehat{\Gamma} \\ &\geq -\ln \mathrm{Tr}\left(\textstyle\sum_\alpha P_\alpha \widehat{\Gamma}\right) \geq -\ln \left\|\textstyle\sum_\alpha P_\alpha\right\| . \end{aligned} \tag{3.18}$$

■

Let $\chi = \max_\alpha \|F^{N_\alpha,M_\alpha}\psi_\alpha\|^{-2}$. Then,

$$\sum_\alpha |\phi_\alpha\rangle\langle\phi_\alpha| \leq \chi \sum_\alpha F^{N_\alpha,M_\alpha}|\psi_\alpha\rangle\langle\psi_\alpha|F^{N_\alpha,M_\alpha}\,. \tag{3.19}$$

Note that F^{N_α,M_α} depends on α only through the particle numbers N_α and M_α. Denoting the sum over a sector of fixed N_α and M_α by $\sum'$, and using the fact that the ψ_α are orthonormal, we see that

$$\textstyle\sum'_\alpha F^{N_\alpha,M_\alpha}|\psi_\alpha\rangle\langle\psi_\alpha|F^{N_\alpha,M_\alpha} \leq |F^{N_\alpha,M_\alpha}|^2 \leq 1\,. \tag{3.20}$$

This hold in every sector, and hence

$$\sum_\alpha |\phi_\alpha\rangle\langle\phi_\alpha| \leq \chi\,. \tag{3.21}$$

Lemma 2 thus implies that

$$S[\Gamma] \geq S[\Gamma_Q] - \ln\chi\,, \tag{3.22}$$

and it remains to derive an upper bound χ. Equivalently, we need a lower bound on the norm $\|F^{N_\alpha,M_\alpha}\psi_\alpha\|$. This can be obtained as follows.

Lemma 3. *Under the same assumptions as in Lemma 1,*

$$\langle\psi|\psi\rangle \geq \left[1 - c\left(\frac{aR^2}{s^3} + s^2 k\right)\right]_+^{\min\{N,M\}} \left[1 - c(N+M)^{8/3}(s/\ell)^5\right]_+ \tag{3.23}$$

for some constant $c > 0$. Here, $[t]_+ = \max\{t, 0\}$ denotes the positive part.

Proof. We write $F^{N,M}(X^\uparrow, X^\downarrow) = G_N(X^\uparrow)G_M(X^\downarrow)H(X^\uparrow, X^\downarrow)$, where G_N, G_M and H denote the three different factors in (3.7). From [4, Lemmas 1 and 3] we can infer that

$$\begin{aligned}
\langle\psi|\psi\rangle &= \int dX^\uparrow\, dX^\downarrow\, D_1(X^\uparrow)^2 D_2(X^\downarrow)^2 G_N(X^\uparrow)^2 G_M(X^\downarrow)^2 H(X^\uparrow, X^\downarrow)^2 \\
&\geq \int dX^\uparrow\, dX^\downarrow\, D_1(X^\uparrow)^2 D_2(X^\downarrow)^2 G_N(X^\uparrow)^2 H(X^\uparrow, X^\downarrow)^2 \\
&\quad \times \left[1 - cM^{8/3}\|\mathbb{A}_{X^\uparrow}^{-1}\|^2 (s/\ell)^5\right]_+ \\
&= \int dX^\uparrow\, D_1(X^\uparrow)^2 G_N(X^\uparrow)^2 \big(\det \mathbb{A}_{X^\uparrow}\big) \left[1 - cM^{8/3}\|\mathbb{A}_{X^\uparrow}^{-1}\|^2 (s/\ell)^5\right]_+ .
\end{aligned} \tag{3.24}$$

Here, $\mathbb{A}_{X^\uparrow}$ denotes the $M \times M$ matrix

$$\left(\mathbb{A}_{X^\uparrow}\right)_{nm} = \int_{\mathbb{R}^3} dy\, \varphi_n^*(y)\varphi_m(y) \prod_{j=1}^N f(y - x_j^\uparrow)^2 \,, \tag{3.25}$$

with φ_n denoting the M eigenfunctions of the Dirichlet Laplacian that constitute the Slater determinant D_2, and $\|\cdot\|$ stands for the operator norm. Note that because of the factor G_N the integrand in (3.24) is only non-zero if $|x_i^\uparrow - x_j^\uparrow| \geq s$ for all $i \neq j$. In this case, Lemma 2 in [4] implies that

$$\|\mathbb{I} - \mathbb{A}_{X^\uparrow}\| \leq c\left(\frac{aR^2}{s^3} + s^2 k\right) . \tag{3.26}$$

(Again, as already mentioned after Lemma 1, the factor $n^{2/3}/\ell^2$ in the statement of [4, Lemma 2] has to be replaced by k in the general case considered here.) In particular, since $0 \leq \mathbb{A} \leq \mathbb{I}$, this estimate implies that

$$\|\mathbb{A}_{X^\uparrow}^{-1}\| \leq \left[1 - c\left(\frac{aR^2}{s^3} + s^2 k\right)\right]_+^{-1} \tag{3.27}$$

and that

$$\det \mathbb{A}_{X^\uparrow} \geq \left[1 - c\left(\frac{aR^2}{s^3} + s^2 k\right)\right]_+^{M} . \tag{3.28}$$

By inserting these two bounds into (3.24) and using again [4, Lemma 3] to get rid of the G_N in the integrand this implies (3.23) in the case $M \leq N$. The case $N > M$ follows in the same way, interchanging the estimates for the $X^\uparrow$ and $X^\downarrow$-particles. ■

To apply this lemma, we use again the fact that in the case of interest the number of particles is at most $N + M \leq 2\,\mathrm{Tr}_{\mathcal{H}_1} Q \leq c\ell^3 K^{3/2}\varrho_0$ for some constant $c > 0$, and the kinetic energy k is bounded by $K\varrho_0^{2/3}$. Hence Lemma 3 implies that

$$\frac{1}{\chi} \geq \left[1 - c\left(\frac{aR^2}{s^3} + s^2 K\varrho_0^{2/3}\right)\right]_+^{c\ell^3 K^{3/2}\varrho_0} \left[1 - c\ell^3 K^4 \varrho_0 \left(s^3\varrho_0\right)^{5/3}\right]_+ \tag{3.29}$$

for some constant $c > 0$. In combination, (3.15), (3.16) and (3.22) imply the lower bound

$$\begin{aligned}\mathcal{P}^\ell[\Gamma] \;\geq\; &\mathcal{P}_0^\ell[\Gamma_Q] - 2\pi a\varrho_Q^2 - \frac{1}{\ell^3\beta}\ln\chi \\ &- ca\varrho_Q^2\left[\ell^{-1}\varrho_Q^{-1/3} + K^2\varrho_0^{4/3}\varrho_Q^{-1}s^{3/2}a^{-1/2} + E\big(R, s, K^{3/2}\varrho_0\ell^3, K\varrho_0^{2/3}, \ell\big)\right] ,\end{aligned} \tag{3.30}$$

with χ bounded by (3.29).

3.4 Approximating Traces by Integrals

The pressure of Γ_Q is easy to compute:

$$\mathcal{P}_0^\ell[\Gamma_Q] = \frac{2}{\beta\ell^3}\mathrm{Tr}_{\mathcal{H}_1}\, \ln\big(1 + Q\exp\big(-\beta(-\Delta-\mu)\big)\big)\,. \tag{3.31}$$

We have to compare this quantity with the true pressure of the non-interacting gas in the thermodynamic limit,

$$P_0(\beta,\mu) = \frac{2}{\beta}(2\pi)^{-3}\int_{\mathbb{R}^3} dp\, \ln\big(1+\exp\big(-\beta(p^2-\mu)\big)\big)\,. \tag{3.32}$$

To this end, we note the following:

Lemma 4. *Let $f:\mathbb{R}_+\mapsto\mathbb{R}_+$ be a monotone decreasing function, and let Δ be the Dirichlet Laplacian on a cube of side length ℓ. Then*

$$(2\pi)^{-3}\int_{\mathbb{R}^3} dp\, f(p^2) \geq \ell^{-3}\mathrm{Tr}_{\mathcal{H}_1}\, f(-\Delta) \geq (2\pi)^{-3}\int_{\mathbb{R}^3} dp\, f(p^2)\left[1-\frac{3\pi}{\ell|p|}\right]\,. \tag{3.33}$$

Proof. Note that the spectrum of $-\Delta$ is given by $[(\pi/\ell)\mathbb{N}]^3$. Considering the trace as a lower Riemann sum to the integral, we immediately obtain the first inequality. To obtain the second, we consider the trace as an upper Riemann sum to the integral over the region where $p_i\geq\pi/\ell$, $1\leq i\leq 3$, with p_i denoting the components of p. Hence

$$(2\pi)^3\ell^{-3}\mathrm{Tr}_{\mathcal{H}_1}\, f(-\Delta) \geq \int_{\mathbb{R}^3} dp\, f(p^2) - \sum_{i=1}^3 8\int_{0\leq p_i\leq\pi/\ell} dp\, f(p^2)\,. \tag{3.34}$$

Since f is monotone decreasing, we can estimate

$$\int_{0\leq p_i\leq\pi/\ell} dp\, f(p^2) \leq \frac{1}{4}\frac{\pi}{\ell}\int_{\mathbb{R}^2} dp\, f(p^2) = \frac{1}{8}\frac{\pi}{\ell}\int_{\mathbb{R}^3} dp\,\frac{1}{|p|}f(p^2)\,, \tag{3.35}$$

where the integral in the second term is over the plane $\mathbb{R}^2$. Combining (3.34) and (3.35) we arrive at the second inequality in (3.33). ■

From this lemma, we immediately see that $\varrho_Q \leq \varrho_0$. Moreover,

$$\mathcal{P}_0^\ell[\Gamma_Q] - P_0(\beta,\mu) \geq -\frac{2}{\beta}(2\pi)^{-3}\int_{p^2\geq K\varrho_0^{2/3}} dp\, \ln\left(1+z\exp(-\beta p^2)\right)$$
$$-\frac{2}{\beta}(2\pi)^{-3}\frac{3\pi}{\ell}\int_{p^2\leq K\varrho_0^{2/3}} dp\, \frac{1}{|p|}\ln\left(1+z\exp(-\beta p^2)\right)\,. \tag{3.36}$$

In the integrand in the first integral, we estimate $\ln(1+x)\leq x$ as well as $|p|\leq(2\beta)^{-1/2}\exp(\frac{1}{2}\beta p^2)$ and obtain

$$\frac{2}{\beta}(2\pi)^{-3}\int_{p^2\geq K\varrho_0^{2/3}} dp\, \ln\left(1+z\exp(-\beta p^2)\right) \leq \frac{1}{\sqrt{2}\pi^2}\frac{z}{\beta^{5/2}}\exp\left(-\tfrac{1}{2}\beta K\varrho_0^{2/3}\right)\,. \tag{3.37}$$

The second term on the right side of (3.36) is bounded from below by

$$-\frac{3}{4\pi^2}\frac{1}{\beta^2\ell}\int_{\mathbb{R}^3} dp\, \frac{1}{|p|}\ln\left(1+z\exp(-p^2)\right) \equiv -\frac{3}{4\pi^2}\frac{1}{\beta^2\ell}g(z)\,, \tag{3.38}$$

and therefore

$$\mathcal{P}_0^\ell[\Gamma_Q] \geq P_0(\beta,\mu) - \frac{1}{\pi^2\beta^{5/2}}\left[\frac{3\beta^{1/2}}{4\ell}g(z) + \frac{z}{\sqrt{2}}\exp\left(-\tfrac{1}{2}\beta K\varrho_0^{2/3}\right)\right]\,. \tag{3.39}$$

By combining (3.39) with (3.30) and the estimate $\varrho_Q\leq\varrho_0$, we thus obtain, for some constant $c>0$,

$$\begin{aligned}P^\ell(\beta,\mu) \;\geq\; & P_0(\beta,\mu) - 2\pi a\varrho_0^2 - \frac{1}{\ell^3\beta}\ln\chi \\ & -ca\varrho_0^2\Big[\ell^{-1}\varrho_0^{-1/3} + K^2\varrho_0^{1/3}s^{3/2}a^{-1/2} + E\big(R,s,K^{3/2}\varrho_0\ell^3,K\varrho_0^{2/3},\ell\big)\Big] \\ & -\frac{1}{\pi^2\beta^{5/2}}\left[\frac{3\beta^{1/2}}{4\ell}g(z) + \frac{z}{\sqrt{2}}\exp\left(-\tfrac{1}{2}\beta K\varrho_0^{2/3}\right)\right]\,,\end{aligned} \tag{3.40}$$

with χ bounded by (3.29).

3.5 Final Result

We are still free to choose ℓ, R, s and K. We choose

$$R = a(a^3\varrho_0)^{-1/81}\ ,\ s = a(a^3\varrho_0)^{-10/81}\ ,\ \ell = \varrho_0^{-1/3}(a^3\varrho_0)^{-28/81} \tag{3.41}$$

and $K = (a^3\varrho_0)^{-\varepsilon/12}$ for some $\varepsilon > 0$. With this choice the first term in square brackets in (3.40) is bounded by

$$\ell^{-1}\varrho_0^{-1/3} + K^2\varrho_0^{1/3}s^{3/2}a^{-1/2} + E\big(R, s, K^{3/2}\varrho_0\ell^3, K\varrho_0^{2/3}, \ell\big) \leq c\big(a\varrho_0^{1/3}\big)^{1/27-\varepsilon} \tag{3.42}$$

for some $c > 0$ and $a^3\varrho_0$ small. Moreover,

$$\frac{1}{\ell^3\beta}\ln\chi \leq \text{const.}\,\frac{1}{\beta\varrho_0^{2/3}}a\varrho_0^2\big(a\varrho_0^{1/3}\big)^{1/27-3\varepsilon/8}\,. \tag{3.43}$$

Note that $\beta\varrho_0^{2/3}$ is a monotone increasing function of z and, in particular, $1/(\beta\varrho_0^{2/3})$ is bounded for bounded $1/z$.

The first term in the last line of (3.40) is

$$\frac{1}{\beta^2\ell}g(z) = a\varrho_0^2\frac{g(z)}{\big(\beta\varrho_0^{2/3}\big)^2}\big(a\varrho_0^{1/3}\big)^{1/27}\,. \tag{3.44}$$

Now $\beta\varrho_0^{2/3} \sim \ln(z)$ for large z, and also $g(z) \sim \ln(z)$ for large z. Hence the fraction in (3.44) is uniformly bounded in z for bounded $1/z$. The remaining term in (3.40) is

$$\varrho_0^{5/3}\frac{1}{\big(\beta\varrho_0^{2/3}\big)^{5/2}}\left[\exp\left(-\tfrac{1}{2}\beta\varrho_0^{2/3} + K^{-1}\ln z\right)\right]^K\,. \tag{3.45}$$

For large K, the term in square brackets is strictly less than one, again uniformly in z. Hence we see that the expression (3.45) is exponentially small for small $a^3\varrho_0$ and, in particular, bounded by const. $\varrho_0^{5/3}(a^3\varrho_0)^p$ for any exponent p, with a constant that depends on p (and ε), of course, but not on z (for bounded $1/z$).

To summarize, we have thus shown that with the choice of parameters as above, (3.40) gives, for any $\varepsilon > 0$,

$$P^\ell(\beta,\mu) \geq P_0(\beta,\mu) - 2\pi a\varrho_0^2\left(1 + C_\varepsilon(z)\big(a\varrho_0^{1/3}\big)^{1/27-\varepsilon}\right)\,, \tag{3.46}$$

with some constant $C_\varepsilon(z)$ that is uniformly bounded in z for bounded $1/z$. To complete the estimate, we have to insert this bound into (3.2). Thus we still have to estimate

$$\frac{R_0}{\ell}P_0(\beta,\mu) = \frac{R_0}{a}a\varrho_0^2\big(a\varrho_0^{1/3}\big)^{28/81}\big(\beta\varrho_0^{2/3}\big)^{-5/2}P_0(1,\beta\mu)\,. \tag{3.47}$$

Now $P_0(1,\beta\mu) \sim (\ln z)^{5/2}$ for large z, and therefore $(\beta\varrho_0^{2/3})^{-5/2}P_0(1,\beta\mu)$ is uniformly bounded for bounded $1/z$. Altogether, this implies that, for some constant $C_\varepsilon(z)$ uniformly bounded for bounded $1/z$,

$$P(\beta,\mu) \geq P_0(\beta,\mu) - 2\pi a\varrho_0^2 \left(1 + C_\varepsilon(z)\big(a\varrho_0^{1/3}\big)^{1/27-\varepsilon}\right) . \tag{3.48}$$

This finishes the proof of the lower bound.

4 Upper Bound to the Pressure

In maximizing the pressure functional we can restrict ourselves to density matrices that do not mix particle numbers. More precisely, if $Q_N^{\updownarrow}$ denotes the projection onto the sector of N particles in $\mathcal{F}_{\updownarrow}$, then $\mathcal{P}^L[\Gamma] \leq \mathcal{P}^L[\widehat{\Gamma}]$, with $\widehat{\Gamma} = \sum_{N,M} Q_N^{\uparrow}Q_M^{\downarrow}\Gamma Q_N^{\uparrow}Q_M^{\downarrow}$. This follows from the fact that the entropy is non-decreasing under this transformation [12, 2.1,11.4]. Hence we can assume that $\Gamma = \bigoplus_{N,M}\Gamma_{N,M}$, with $\Gamma_{N,M}$ (not normalized) density matrices for N $\uparrow$-particles and M $\downarrow$-particles, respectively. For simplicity, we may also assume that Γ is symmetric with respect to exchange of $\uparrow$ and $\downarrow$. This is certainly no restriction in the case considered here, and leads to simpler expressions by shortening some of the formulas.

4.1 Lower Bound to the Hamiltonian

We start with a lemma which is essentially a generalization of a result by Dyson [1] to bound the hard potential v from below by a soft potential U, at the expense of some kinetic energy. In the following, $\widehat{f}$ denotes the Fourier transform of a function f. We use the convention $\widehat{f}(p) = (2\pi)^{-3/2}\int dx\, f(x)e^{-ipx}$.

Lemma 5. *Let χ be a radial function, $0 \leq \chi \leq 1$, with $h \equiv \widehat{1-\chi} \in L^1(\mathbb{R}^3)\cap L^\infty(\mathbb{R}^3)$. For $R > R_0$, let*

$$f_R(x) = \sup_{|y|\leq R} |h(x-y) - h(x)| , \tag{4.1}$$

and

$$w_R(x) = \frac{2}{\pi^2} f_R(x) \int_{\mathbb{R}^3} dy\, f_R(y) . \tag{4.2}$$

Let U be a positive, radial function, supported in the annulus $R_0 \leq |x| \leq R$, with $\int_{\mathbb{R}^3} dx\, U(x) = 4\pi$. If $y_1, \ldots, y_M$ denotes a set of M points in $\mathbb{R}^3$, with

$|y_k - y_l| \geq 2R$ for all $k \neq l$, then, for any $\varepsilon > 0$,

$$-\nabla\chi(p)^2\nabla + \tfrac{1}{2}\sum_{k=1}^{M} v(x-y_k) \geq \sum_{k=1}^{M}\Big((1-\varepsilon)aU(x-y_k) - \frac{a}{\varepsilon}w_R(x-y_k)\Big) \tag{4.3}$$

in the sense of quadratic forms. Here, $\chi(p)$ stands for the multiplication operator in momentum space. This operator inequality holds for all functions in $H^1(\mathbb{R}^3)$ and therefore, in particular, for functions supported in the cube Λ_L.

The proof of this lemma can be found in [4, Lemma 4 and Cor. 1]. Note that, by construction, either $w_R \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, or $w_R \equiv \infty$ identically.

Lemma 5 implies the following lower bound to the Hamiltonians (2.1):

$$\begin{aligned} H_{N,M} \;\geq\; & \sum_{i=1}^{N}\Big[-\nabla_i^\uparrow\Big(1-\chi(p_i^\uparrow)^2\Big)\nabla_i^\uparrow + W_{X^\downarrow}(x_i^\uparrow)\Big] \\ & + \sum_{k=1}^{M}\Big[-\nabla_k^\downarrow\Big(1-\chi(p_k^\downarrow)^2\Big)\nabla_k^\downarrow + W_{X^\uparrow}(x_k^\downarrow)\Big] \,. \end{aligned} \tag{4.4}$$

Here, W_Y is the potential

$$W_Y(x) = \sum_{\{k\,:\,y_k\in\widetilde{Y}_R\}}\Big((1-\varepsilon)aU(x-y_j) - \frac{a}{\varepsilon}w_R(x-y_j)\Big)\,, \tag{4.5}$$

where $Y = (y_1,\ldots,y_M)$ is any set of coordinates in Λ_L and $\widetilde{Y}_R \subset Y$ is the subset of y_j's whose distance to the nearest neighbor in Y is at least $2R$. We neglect the interaction with y_j's that are not in the set $\widetilde{Y}_R$, which can only lower the energy. Note that also the interaction terms among particles of equal spin are dropped for a lower bound.

The expectation value of the potentials $W_{X^\uparrow}$ and $W_{X^\downarrow}$ can be written in the following convenient way. For $\Gamma = \bigoplus_{N,M}\Gamma_{N,M}$ a density matrix on $\mathcal{F}_\uparrow \otimes \mathcal{F}_\downarrow$, and $X^\downarrow = (x_1^\downarrow,\ldots,x_M^\downarrow)$ some fixed coordinates of the spin-down particles, let the operator $\Gamma_N^{X^\downarrow}$ be defined through the integral kernel $\Gamma_N^{X^\downarrow}(X^\uparrow, Y^\uparrow) = \Gamma_{N,M}(X^\uparrow, X^\downarrow, Y^\uparrow, X^\downarrow)$. Since $\Gamma_{N,M}$ is a trace class operator, this expression is well defined for almost every $X^\downarrow$ by an eigenfunction expansion of $\Gamma_{N,M}$. The same is true for $n(X^\downarrow)$, given by $n(X^\downarrow) = \mathrm{Tr}_{\mathcal{F}_\uparrow}[\bigoplus_N \Gamma_N^{X^\downarrow}]$. Note that $n(X^\downarrow)$ is the probability density for having exactly M spin-down particles at the positions $X^\downarrow$. In case $n(X^\downarrow) > 0$, let

$$\Gamma_\uparrow^{X^\downarrow} = n(X^\downarrow)^{-1}\bigoplus_N \Gamma_N^{X^\downarrow}\,. \tag{4.6}$$

This defines $\Gamma_{\uparrow}^{X^{\downarrow}}$ only if $n(X^{\downarrow})$ is non-zero; only in this case it will be used below, however. Note that $\Gamma_{\uparrow}^{X^{\downarrow}}$ is a density matrix on $\mathcal{F}_{\uparrow}$, which can be interpreted as the density matrix of the $\uparrow$-particles for a fixed configuration of the $\downarrow$-particles. If $\gamma_{\uparrow}^{X^{\downarrow}}$ denotes the reduced one-particle density matrix of $\Gamma_{\uparrow}^{X^{\downarrow}}$, then the expectation value of the potential $W_{X^{\downarrow}}$ in the state Γ can be written as

$$\sum\!\!\!\!\!\!\!\int dX^{\downarrow}\, n(X^{\downarrow})\,\mathrm{Tr}_{\mathcal{H}_1}\left[W_{X^{\downarrow}}\gamma_{\uparrow}^{X^{\downarrow}}\right] , \tag{4.7}$$

where we introduced the short hand notation $\sum\!\!\!\!\!\!\int dX^{\downarrow} \equiv \sum_M \int dx_1^{\downarrow}\cdots dx_M^{\downarrow}$. Note that $\sum\!\!\!\!\!\!\int dX^{\downarrow}\, n(X^{\downarrow}) = 1$, and $\sum\!\!\!\!\!\!\int dX^{\downarrow}\, n(X^{\downarrow})\,\Gamma_{\uparrow}^{X^{\downarrow}} = \Gamma_{\uparrow} \equiv \mathrm{Tr}_{\mathcal{F}_{\downarrow}}\Gamma$.

Under the assumption that the density matrix is symmetric with respect to exchange of $\uparrow$ and $\downarrow$-particles, the lower bound to the Hamiltonian in (4.4) can thus be written as follows:

$$\mathrm{Tr}_{\mathcal{F}}\, H\Gamma \geq 2\sum\!\!\!\!\!\!\!\int dX^{\downarrow}\, n(X^{\downarrow})\,\mathrm{Tr}_{\mathcal{H}_1}\left[\big(-\nabla(1-\chi(p)^2)\nabla + W_{X^{\downarrow}}\big)\gamma_{\uparrow}^{X^{\downarrow}}\right] . \tag{4.8}$$

Note that the kinetic energy term does not depend on $X^{\downarrow}$ and, therefore, the integration affects only $\gamma_{\uparrow}^{X^{\downarrow}}$. Note also that $\sum\!\!\!\!\!\!\int dX^{\downarrow}\, n(X^{\downarrow})\,\gamma_{\uparrow}^{X^{\downarrow}} = \gamma_{\uparrow}$, the reduced one-particle density matrix for the $\uparrow$-particles.

For reasons which will become clear later, we find it convenient not to use up all the kinetic energy in the bound (4.8), however. More precisely, we pick some $0<\delta<1$ and $0<\varkappa<1$ and write $-\Delta$ as

$$-\Delta = -\delta\Delta - (1-\delta)(1-\varkappa)\nabla\chi(p)^2\nabla + h^{\chi} , \tag{4.9}$$

with

$$h^{\chi} = -(1-\delta)\nabla\big(1-(1-\varkappa)\chi(p)^2\big)\nabla . \tag{4.10}$$

Applying the above estimate only to the second term on the right side of (4.9) and using positivity of the interaction potential v, we obtain that

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}}\, H\Gamma \;\geq\; & 2\,\mathrm{Tr}_{\mathcal{H}_1}\left[\big(-\delta\Delta + h^{\chi}\big)\gamma_{\uparrow}\right] \\ & +2(1-\delta)(1-\varkappa)\sum\!\!\!\!\!\!\!\int dX^{\downarrow}\, n(X^{\downarrow})\,\mathrm{Tr}_{\mathcal{H}_1}\left[W_{X^{\downarrow}}\gamma_{\uparrow}^{X^{\downarrow}}\right] . \end{aligned} \tag{4.11}$$

Eq. (4.11) is the final result of this subsection. To estimate this expression, we will show that, for any fixed $X^{\downarrow}$, the one-particle density matrix $\gamma_{\uparrow}^{X^{\downarrow}}$ is close to the corresponding expression for non-interacting particles (which does not depend on $X^{\downarrow}$, of course). We do this in Subsection 4.3 below.

It remains to choose χ. Let $\eta : \mathbb{R}^3 \to \mathbb{R}_+$ be a smooth radial function with $\eta(x) = 0$ for $|x| \leq 1$, $\eta(x) = 1$ for $|x| \geq 2$, and $0 \leq \eta(x) \leq 1$ in-between. For some $s > 0$ we choose

$$\chi(p) = \eta(sp)\,. \tag{4.12}$$

The potential W_Y then depends on ε, a, R and s. Note that with this choice of χ the corresponding $h = \widehat{1-\chi}$ is a smooth function of rapid decay and hence, by simple scaling, the corresponding potential w_R defined in (4.2) satisfies, for $R \leq \text{const.}\, s$,

$$\|w_R\|_\infty \leq \text{const.}\, \frac{R^2}{s^5} \quad \text{and} \quad \|w_R\|_1 \leq \text{const.}\, \frac{R^2}{s^2} \tag{4.13}$$

for some constants depending only on η, which is fixed once and for all. Moreover, if $|y_k - y_l| \geq 2R$ for all $k \neq l$, then

$$\sum_{k=1}^{M} w_R(x - y_k) \leq \text{const.}\, \frac{1}{Rs^2} \tag{4.14}$$

independently of x and M.

We are also still free to choose the potential U in Lemma 5. We choose

$$U(x) = \begin{cases} 3\left(R^3 - R_0^3\right)^{-1} & \text{for } R_0 \leq |x| \leq R, \\ 0 & \text{otherwise}\,. \end{cases} \tag{4.15}$$

We then have the estimate

$$\|W_Y\|_\infty \leq \max\left\{ \frac{3a}{R^3 - R_0^3}\,,\ \text{const.}\, \frac{a}{\varepsilon R s^2} \right\}, \tag{4.16}$$

independently of Y.

4.2 Improved Subadditivity of Entropy

For Γ a density matrix on $\mathcal{F}_\uparrow \otimes \mathcal{F}_\downarrow$, let $\Gamma_\uparrow = \operatorname{Tr}_{\mathcal{F}_\downarrow} \Gamma$ and $\Gamma_\downarrow = \operatorname{Tr}_{\mathcal{F}_\uparrow} \Gamma$ be the density matrices of the subsystems of $\uparrow$ and $\downarrow$-particles, respectively. It is well known that the entropy $S[\Gamma]$ is subadditive (see, e.g., [12, Ineq. (2.2,13)], i.e.,

$$S[\Gamma] \leq S[\Gamma_\uparrow] + S[\Gamma_\downarrow]\,, \tag{4.17}$$

where the entropies on the right side are defined by taking the trace only over $\mathcal{F}_\uparrow$ and $\mathcal{F}_\downarrow$, respectively. Moreover, if $\gamma_\updownarrow$ denotes the reduced one-particle density matrix of $\Gamma_\updownarrow$, then

$$S[\Gamma_\updownarrow] \leq \widetilde{S}[\gamma_\updownarrow]\,, \tag{4.18}$$

where $\widetilde{S}[\gamma] = \mathrm{Tr}_{\mathcal{H}_1}(-\gamma\ln\gamma - (1-\gamma)\ln(1-\gamma))$ is given as in (2.5) [12, Ineq. (2.5,18.5)]. Note that both (4.17) and (4.18) are equalities if Γ is the grand-canonical Gibbs density matrix of a non-interacting system.

We are going to need the following refinement of subadditivity of entropy. Its proof is given in [3, Cor. 4].

Lemma 6. *Let $\Gamma = \bigoplus_{N,M}\Gamma_{N,M}$ be a density matrix on $\mathcal{F}_\uparrow\otimes\mathcal{F}_\downarrow$. With the notation introduced in Subsect. 4.1,*

$$S[\Gamma] \le S[\Gamma_\downarrow] + \sum\!\!\!\!\!\!\int dX^\downarrow\, n(X^\downarrow)\, S[\Gamma_\uparrow^{X^\downarrow}]\,. \tag{4.19}$$

Note that $\sum\!\!\!\!\!\!\int dX^\downarrow\, n(X^\downarrow) = 1$, and $\sum\!\!\!\!\!\!\int dX^\downarrow\, n(X^\downarrow)\Gamma_\uparrow^{X^\downarrow} = \Gamma_\uparrow$. Hence, by concavity of $S[\Gamma_\uparrow]$, inequality (4.19) is stronger than the usual subadditivity of entropy in (4.17). The last term on the right side of (4.19) is the average entropy of the $\uparrow$-particles for fixed $\downarrow$-particles, whereas $S[\Gamma_\uparrow]$ is the entropy of the state of $\uparrow$-particles averaged over all configurations of the $\downarrow$-particles.

4.3 A Priori Bounds on the One-Particle Density Matrix

In this subsection we will show that the one-particle density matrices for fixed $\downarrow$-particles, $\gamma_\uparrow^{X^\downarrow}$, are close to the corresponding expression for non-interacting particles, provided the state Γ that defines them has a variational pressure $\mathcal{P}^L[\Gamma]$ close to the true pressure $P^L(\beta,\mu)$ of the system, i.e., it is an approximate maximizer of the pressure functional (2.2) in a sense to be made precise below. We call such a bound an *a priori* bound.

This subsection is split into four parts. In Part 1, we will derive a bound of the sort needed. This bound will not be uniform in the fugacity z, however, and will be useless for very large z (when the system is close to its ground state). For large z, however, we will use a different method to obtain a similar bound, by comparing the state with the ground state of the non-interacting system. We do this in Part 3. Before that, we use the method of Part 1 to compare the non-interacting system with different boundary conditions (Part 2). Some calculations are easier to do with periodic boundary conditions than with Dirichlet, hence the usefulness of this estimate. Finally, we give a summary of the result of this subsection in Part 4.

4.3.1 General a priori bound

Using the fact that $v \geq 0$, we can infer from Lemma 6 and (4.18) that

$$
\begin{aligned}
-L^3 \mathcal{P}^L[\Gamma] \geq\ & \mathrm{Tr}_{\mathcal{H}_1}\left[(-\Delta-\mu)\,\gamma_\downarrow\right] - \frac{1}{\beta}\widetilde{S}[\gamma_\downarrow] \\
& + \sum\!\!\!\!\!\!\!\int dX^\downarrow\, n(X^\downarrow)\left(\mathrm{Tr}_{\mathcal{H}_1}\left[(-\Delta-\mu)\,\gamma_\uparrow^{X^\downarrow}\right] - \frac{1}{\beta}\widetilde{S}\left[\gamma_\uparrow^{X^\downarrow}\right]\right)
\end{aligned} \tag{4.20}
$$

The term in the first line on the right side of (4.20) is bounded from below by $-\frac{1}{2}L^3 P_0^L(\beta,\mu)$ because of (2.4). The same is true for the term in the last line, but we will need a refinement of this inequality, given in Lemma 7 below.

For Γ an approximate maximizer of $\mathcal{P}^L[\Gamma]$, we have an upper bound on the left side of (4.20), derived in the previous section, and therefore this yields an upper bound on the last expression on the right side of (4.20). This bound can be used to get information on the one-particle density matrices $\gamma_\uparrow^{X^\downarrow}$. We need the following lemma.

Lemma 7. *Let h be a self-adjoint operator on a Hilbert space $\mathcal{H}$, such that e^{-h} is trace class. For γ a fermionic one-particle density matrix (i.e., a trace class operator on $\mathcal{H}$ with $0 \leq \gamma \leq 1$), define the functional*

$$\mathcal{E}_h[\gamma] = \mathrm{Tr}\, h\gamma - \widetilde{S}[\gamma]\,. \tag{4.21}$$

Let $\gamma_h = (1+e^h)^{-1}$ be its minimizer, and $f(h) = \mathcal{E}_h[\gamma_h] = -\mathrm{Tr}\ \ln(1+e^{-h})$. Then, for any γ,

$$\mathcal{E}_h[\gamma] \geq f(h) + 2\,\mathrm{Tr}(\gamma-\gamma_h)^2\,, \tag{4.22}$$

and also

$$\mathcal{E}_h[\gamma] \geq f(h) + \frac{1}{2}\frac{|\mathrm{Tr}(\gamma-\gamma_h)|^2}{|\mathrm{Tr}(\gamma-\gamma_h)| + \mathrm{Tr}\,\gamma_h}\,. \tag{4.23}$$

Note that this lemma implies, in particular, that $\gamma \to \gamma_h$ in trace class norm, if $\mathcal{E}_h[\gamma] \to f(h)$. Eq. (4.22) implies convergence in Hilbert-Schmidt norm, but because of (4.23) also the traces converge, and therefore the convergence is in trace class norm (see [13, 11] or Ineq. (4.35) below).

Proof. We write

$$\mathcal{E}_h[\gamma] - f(h) = \mathrm{Tr}\, g(\gamma,\gamma_h)\,, \tag{4.24}$$

with

$$g(\gamma,\gamma_h) = \gamma\ln\gamma - \gamma\ln\gamma_h + (1-\gamma)\ln(1-\gamma) - (1-\gamma)\ln(1-\gamma_h)\,. \tag{4.25}$$

The function g has the integral representation (for $0 \leq x, y \leq 1$)

$$g(x,y) = \int_y^x dz\,(x-z)\left(\frac{1}{z} + \frac{1}{1-z}\right) . \tag{4.26}$$

Using that $1/z + 1/(1-z) \geq 4$ in the integrand, we obtain the lower bound $g(x,y) \geq 2(x-y)^2$. Hence, by Klein's inequality [12, Ineq. (2.1,7.5)], $\mathrm{Tr}\, g(\gamma, \gamma_h) \geq 2\,\mathrm{Tr}(\gamma - \gamma_h)^2$, and (4.22) follows. Moreover, estimating $1/z + 1/(1-z) \geq 1/z \geq 1/\max\{x,y\} \geq 1/(|x-y|+y)$ in the integrand in (4.26), we obtain

$$g(x,y) \geq \frac{1}{2}\frac{(x-y)^2}{|x-y|+y} = 2 \sup_{0<b<1} \left[b(1-b)|x-y| - b^2 y\right] . \tag{4.27}$$

Hence, again by Klein's inequality,

$$\mathrm{Tr}\, g(\gamma, \gamma_h) \geq 2b(1-b)|\mathrm{Tr}(\gamma - \gamma_h)| - 2b^2 \mathrm{Tr}\,\gamma_h \tag{4.28}$$

for any $0 < b < 1$. Taking the supremum over b yields (4.23). ■

We now apply this lemma to (4.20), with $h = \beta(-\Delta - \mu)$. Note that $f(h) = -\frac{1}{2}\beta L^3 P_0^L(\beta,\mu)$ in this case. Let $\gamma_0 = \gamma_h = (1 + z^{-1}\exp(-\beta\Delta))^{-1}$ be the minimizer of (4.21). We can infer from (4.22) and (4.20) that

$$\sum\!\!\!\!\!\!\int dX^{\downarrow}\, n(X^{\downarrow})\,\mathrm{Tr}\big(\gamma_{\uparrow}^{X^{\downarrow}} - \gamma_0\big)^2 \leq \tfrac{1}{2}\beta L^3 \left(P_0^L(\beta,\mu) - \mathcal{P}^L[\Gamma]\right) . \tag{4.29}$$

If L is large, $a^3\varrho_0$ small, and $z = e^{\beta\mu}$ is bounded away from zero, the lower bound to the pressure derived in the previous section shows that we can restrict our attention to density matrices Γ with $\mathcal{P}^L[\Gamma] \geq P_0^L(\beta,\mu) - Ca\varrho_0^2$, for some constant $C > 2\pi$. Hence, for such a Γ,

$$\sum\!\!\!\!\!\!\int dX^{\downarrow}\, n(X^{\downarrow})\,\mathrm{Tr}\big(\gamma_{\uparrow}^{X^{\downarrow}} - \gamma_0\big)^2 \leq \tfrac{1}{2}C\beta L^3 a\varrho_0^2 . \tag{4.30}$$

Using (4.23) instead of (4.22), we obtain in the same way

$$\sum\!\!\!\!\!\!\int dX^{\downarrow}\, n(X^{\downarrow})\,\frac{\left|\mathrm{Tr}\big(\gamma_{\uparrow}^{X^{\downarrow}} - \gamma_0\big)\right|^2}{\left|\mathrm{Tr}\big(\gamma_{\uparrow}^{X^{\downarrow}} - \gamma_0\big)\right| + \mathrm{Tr}\,\gamma_0} \leq 2C\beta L^3 a\varrho_0^2 . \tag{4.31}$$

By using convexity of the map $x \mapsto x^2/(x+1)$, as well as the fact that, by Lemma 4, $\mathrm{Tr}\,\gamma_0 \leq \frac{1}{2}L^3\varrho_0$, (4.31) implies that

$$\sum\!\!\!\!\!\!\int dX^{\downarrow}\, n(X^{\downarrow})\,\left|\mathrm{Tr}\big(\gamma_{\uparrow}^{X^{\downarrow}} - \gamma_0\big)\right| \leq L^3\varrho_0\sqrt{Ca\varrho_0\beta}\left(1 + \sqrt{4Ca\varrho_0\beta}\right) . \tag{4.32}$$

We thus have an upper bound on both the average Hilbert-Schmidt norm of the difference of $\gamma_\uparrow^{X\downarrow}$ and γ_0 and the average difference of their trace. We can thus obtain a bound on the average trace norm of their difference, which will be needed in the next subsection.

Let a and b be two positive trace class operators, let P be a projection with finite rank, and set $Q = 1 - P$. With $\|\cdot\|_p = (\mathrm{Tr}[|\cdot|^p])^{1/p}$ denoting the Schatten p-norm, we have

$$\begin{aligned} \|a-b\|_1 &\leq \|(a-b)P\|_1 + \|aQ\|_1 + \|bQ\|_1 \\ &\leq \|P\|_2\|a-b\|_2 + \|a\|_1^{1/2}\|QaQ\|_1^{1/2} + \|b\|_1^{1/2}\|QbQ\|_1^{1/2} \,. \end{aligned} \tag{4.33}$$

The trace norm of a can be estimated by $\|a\|_1 \leq \|b\|_1 + |\mathrm{Tr}\,(a-b)|$. Moreover,

$$\begin{aligned} \|QaQ\|_1 &= \mathrm{Tr}\, aQ = \mathrm{Tr}\,[bQ + (a-b) + (a-b)P] \\ &\leq \|QbQ\|_1 + |\mathrm{Tr}(a-b)| + \|P\|_2\|a-b\|_2 \,. \end{aligned} \tag{4.34}$$

In conclusion, we thus obtain that

$$\begin{aligned} \|a-b\|_1 \leq \|P\|_2\|a-b\|_2 + 2\big(\|b\|_1 + |\mathrm{Tr}\,(a-b)|\big)^{1/2} \\ \times\big(\|QbQ\|_1 + |\mathrm{Tr}(a-b)| + \|P\|_2\|a-b\|_2\big)^{1/2} \,. \end{aligned} \tag{4.35}$$

We apply this inequality, with $a = \gamma_\uparrow^{X\downarrow}$ and $b = \gamma_0$, using the estimates (4.30) and (4.32). We choose P to be the projection onto the subspace of $\mathcal{H}_1 = L^2(\Lambda_L;\mathbb{C})$ where $-\Delta \leq K\varrho_0^{2/3}$ for some $K > 0$. Using Lemma 4, we have $\|b\|_1 = \mathrm{Tr}\,\gamma_0 \leq \frac{1}{2}L^3\varrho_0$. Moreover, again by Lemma 4, we can estimate

$$\|P\|_2^2 = \mathrm{Tr}\,P \leq \frac{L^3}{(2\pi)^3}\int dp\,\theta(K\varrho_0^{2/3} - p^2) = L^3\varrho_0\frac{K^{3/2}}{6\pi^2} \tag{4.36}$$

and also

$$\begin{aligned} \|QbQ\|_1 &= \mathrm{Tr}\,Qb \leq z\,\mathrm{Tr}\,e^{\beta\Delta}\theta(-\Delta - K\varrho_0^{2/3}) \\ &\leq z\exp\big(-\tfrac{1}{2}\beta K\varrho_0^{2/3}\big)\mathrm{Tr}\,e^{\frac{1}{2}\beta\Delta} \leq L^3\varrho_0\frac{z\exp\big(-\frac{1}{2}\beta K\varrho_0^{2/3}\big)}{(2\pi\beta)^{3/2}\varrho_0} \,. \end{aligned} \tag{4.37}$$

Similarly to the discussion of the term (3.45) in the calculation of the lower bound, this last fraction is exponentially small in $a^3\varrho_0$ if we choose $K = (a^3\varrho_0)^{-\nu}$ for some $\nu > 0$, uniformly in z for bounded $1/z$. By using (4.30),

(4.32) and (4.35)–(4.37), as well as the Schwarz inequality for the integration over $X^\downarrow$, we infer that, for small $a^3\varrho$ and z bounded away from zero,

$$\sum\!\!\!\!\!\!\!\int dX^\downarrow\, n(X^\downarrow)\, \left\| \gamma_\uparrow^{X^\downarrow} - \gamma_0 \right\|_1 \le C_\nu L^3 \varrho_0 \big(a\varrho_0^{1/3}\big)^{1/4-3\nu/8} \big(\beta\varrho_0^{2/3}\big)^{1/4} \tag{4.38}$$

for some constant C_ν depending on ν.

4.3.2 Comparing different boundary conditions

In the following, it will be convenient to compare $\gamma_\uparrow^{X^\downarrow}$ not with γ_0 but rather with $\gamma_{\rm per}$, which is the minimizer of (4.21) with $h = \beta(-\Delta_{\rm per} - \mu)$, $\Delta_{\rm per}$ denoting the Laplacian with *periodic boundary conditions* on the cube Λ_L. Note that $\gamma_{\rm per}$ has a strictly constant density. The density matrices γ_0 and $\gamma_{\rm per}$ agree in the thermodynamic limit, however. This can be seen as follows. Since the quadratic form domain of Δ is included in the quadratic form domain of $\Delta_{\rm per}$, we can use γ_0 as a trial density matrix of $\mathcal{E}_h$ with $h = \beta(-\Delta_{\rm per} - \mu)$. Since the pressure is independent of boundary conditions in the thermodynamic limit,

$$\lim_{L\to\infty} \frac{1}{L^3} \Big(f\big(\beta(-\Delta_{\rm per} - \mu)\big) - f\big(\beta(-\Delta - \mu)\big)\Big) = 0\,. \tag{4.39}$$

Thus Lemma 7 together with (4.35) implies that, for fixed β and μ,

$$\lim_{L\to\infty} \frac{1}{L^3} \|\gamma_0 - \gamma_{\rm per}\|_1 = 0\,. \tag{4.40}$$

4.3.3 A bound uniform in the fugacity

The estimate (4.38) is not uniform in the fugacity $z = e^{\beta\mu}$. In fact, $\beta\varrho_0^{2/3}$ grows like $\ln(z)$ for large z. Note that large z corresponds to the low-temperature limit where the system approaches its ground state. Hence, for large z, we will compare $\gamma_\uparrow^{X^\downarrow}$ with the Fermi sea corresponding to the ground state, namely $P_\mu \equiv \theta(\mu + \Delta)$. More precisely, we are going to use (4.38) only in the case when $\beta\varrho_0^{2/3} \le (a^3\varrho_0)^{-1/9}$. For the case of larger z, where $\beta\varrho_0^{2/3} > (a^3\varrho_0)^{-1/9}$, we now derive a separate bound.

We start with the following estimate. Let $Q_\mu = 1 - P_\mu$ and $e(\mu) = \operatorname{Tr}(-\Delta - \mu)P_\mu$. For non-negative numbers $r, s \ge 0$, and for any operator γ with $0 \le \gamma \le 1$,

$$\begin{aligned} &\operatorname{Tr}(-\Delta - \mu + rP_\mu - sQ_\mu)\gamma \\ &\ge \operatorname{Tr}(-\Delta - \mu + rP_\mu - sQ_\mu)\theta(\mu + \Delta - rP_\mu + sQ_\mu) \\ &= e(\mu - r) + e(\mu + s) - e(\mu) + s \operatorname{Tr} P_\mu\,. \end{aligned} \tag{4.41}$$

Hence

$$
\begin{aligned}
&\operatorname{Tr}(-\Delta-\mu)\gamma - e(\mu) \\
&\geq \left[e(\mu-r)-e(\mu)-r\operatorname{Tr}P_\mu\right]+\left[e(\mu+s)-e(\mu)+s\operatorname{Tr}P_\mu\right] \\
&\quad + r\operatorname{Tr}P_\mu(1-\gamma)+s\operatorname{Tr}(1-P_\mu)\gamma\,.
\end{aligned} \tag{4.42}
$$

Note that, in the thermodynamic limit (and for $\mu\geq 0$),

$$
\begin{aligned}
\lim_{L\to\infty}\frac{1}{L^3}\left[e(\mu-r)-e(\mu)-r\operatorname{Tr}P_\mu\right] &= \frac{1}{6\pi^2}\left[-\frac{2}{5}[\mu-r]_+^{5/2}+\frac{2}{5}\mu^{5/2}-r\mu^{3/2}\right] \\
&\geq -\frac{1}{8\pi^2}\mu^{1/2}r^2
\end{aligned} \tag{4.43}
$$

for $r\geq 0$. Similarly, for $s\geq 0$,

$$
\lim_{L\to\infty}\frac{1}{L^3}\left[e(\mu+s)-e(\mu)+s\operatorname{Tr}P_\mu\right]\geq -\frac{1}{8\pi^2}\mu^{1/2}s^2\left(1+\frac{s}{\mu}\right)^{1/2}. \tag{4.44}
$$

Now if we choose $r=4\pi^2\mu^{-1/2}L^{-3}\operatorname{Tr}P_\mu(1-\gamma)$ and $s=0$, (4.42) implies that

$$
\operatorname{Tr}(-\Delta-\mu)\gamma\geq e(\mu)+2\pi^2\mu^{-1/2}L^{-3}\left[\operatorname{Tr}P_\mu(1-\gamma)\right]^2-o(L^3) \tag{4.45}
$$

for any $0\leq\gamma\leq 1$. On the other hand, choosing $r=0$ and

$$
s=\frac{4\pi^2}{L^3}\frac{\operatorname{Tr}(1-P_\mu)\gamma}{\mu^{1/2}+2\pi^{-1/3}L^{-1}\left(\operatorname{Tr}(1-P_\mu)\gamma\right)^{1/3}}\,, \tag{4.46}
$$

a simple estimate yields

$$
\operatorname{Tr}(-\Delta-\mu)\gamma\geq e(\mu)+\frac{\pi^2}{L^3}\frac{\left[\operatorname{Tr}(1-P_\mu)\gamma\right]^2}{\mu^{1/2}+2\pi^{-1/3}L^{-1}\left(\operatorname{Tr}(1-P_\mu)\gamma\right)^{1/3}}-o(L^3)\,. \tag{4.47}
$$

Using (2.4), we have

$$
\operatorname{Tr}(-\Delta-\mu)\gamma-\frac{1}{\beta}\widetilde{S}[\gamma]\geq-\frac{L^3}{4}P_0^L(\beta/2,\mu)+\frac{1}{2}\operatorname{Tr}(-\Delta-\mu)\gamma\,. \tag{4.48}
$$

We use this estimate, together with (4.45), on the last term on the right side of (4.20), with $\gamma=\gamma_\uparrow^{X\downarrow}$. We restrict our attention again to states with $\mathcal{P}^L[\Gamma]\geq P_0^L(\beta,\mu)-Ca\varrho_0^2$ as above. Note that $e(\mu)=-\frac{1}{2}L^3P_0^L(\infty,\mu)$. Let $\Delta P_0^L(\beta,\mu)$ denote the expression

$$
\Delta P_0^L(\beta,\mu)\equiv-2P_0^L(\beta,\mu)+P_0^L(\beta/2,\mu)+P_0^L(\infty,\mu)\geq 0\,. \tag{4.49}
$$

The positivity follows from convexity of $P_0^L(\beta,\mu)$ in $1/\beta$. From (4.20), (4.48) and (4.45) we obtain

$$\frac{1}{L^6}\sum\!\!\!\!\!\!\int dX^\downarrow\, n(X^\downarrow)\,\Big[\mathrm{Tr}\, P_\mu\big(1-\gamma_\uparrow^{X^\downarrow}\big)\Big]^2 \leq \frac{\mu^{1/2}}{4\pi^2}\left(4Ca\varrho_0^2+\Delta P_0^L(\beta,\mu)\right)+o(1)\,. \tag{4.50}$$

By repeating this argument, this time with (4.47) in place of (4.45), and using convexity of the map $x\mapsto x^2/(1+x^{1/3})$, we also obtain the bound

$$\frac{\left[\frac{1}{L^3}\sum\!\!\!\!\!\!\int dX^\downarrow\, n(X^\downarrow)\,\mathrm{Tr}\,(1-P_\mu)\gamma_\uparrow^{X^\downarrow}\right]^2}{1+2\pi^{-1/3}\mu^{-1/2}\left[\frac{1}{L^3}\sum\!\!\!\!\!\!\int dX^\downarrow\, n(X^\downarrow)\,\mathrm{Tr}\,(1-P_\mu)\gamma_\uparrow^{X^\downarrow}\right]^{1/3}} \leq \frac{\mu^{1/2}}{2\pi^2}\left(4Ca\varrho_0^2+\Delta P_0^L(\beta,\mu)\right)+o(1)\,. \tag{4.51}$$

We claim that

$$\Delta P_0^L(\beta,\mu)\leq \frac{2}{3\pi^2}\frac{\mu^{1/2}}{\beta^2}\left(1+\frac{1}{\beta\mu}\right)+o(1) \tag{4.52}$$

in the thermodynamic limit. To see this, first note that $\Delta P_0^L(\beta,\mu)\leq P_0^L(\beta/2,\mu)-P_0^L(\infty,\mu)$. Moreover,

$$\lim_{L\to\infty}\left[P_0^L(\beta,\mu)-P_0^L(\infty,\mu)\right] = \frac{1}{(2\pi)^3\beta}\int_{p^2\leq\mu}dp\,\ln\left(1+z^{-1}e^{\beta p^2}\right) + \frac{1}{(2\pi)^3\beta}\int_{p^2\geq\mu}dp\,\ln\left(1+ze^{-\beta p^2}\right)\,. \tag{4.53}$$

Estimating $\ln(1+x)\leq x$, we see that the first integral is bounded by

$$\frac{4\pi}{3}\frac{\mu^{1/2}}{z}\int_0^{\mu^{1/2}}dp\,pe^{\beta p^2} = \frac{2\pi}{3}\frac{\mu^{1/2}}{\beta}\frac{z-1}{z}\leq \frac{2\pi}{3}\frac{\mu^{1/2}}{\beta}\,. \tag{4.54}$$

In a similar way, the second integral is bounded by

$$\frac{4\pi}{3}\frac{z}{\mu^{1/2}}\int_{\mu^{1/2}}^\infty dp\,p^3e^{-\beta p^2} = \frac{2\pi}{3}\frac{\mu^{1/2}}{\beta}\left(1+\frac{1}{\beta\mu}\right)\,. \tag{4.55}$$

Hence we arrive at (4.52).

Now assume, as explained above, that $\beta\varrho_0^{2/3} > (a^3\varrho_0)^{-1/9}$. For small $a^3\varrho_0$, this means that z has to be large. In this case,

$$\frac{\mu^{1/2}}{2\pi^2}\left(4Ca\varrho_0^2 + \Delta P_0^L(\beta,\mu)\right) \leq \text{const.}\ \varrho_0^2\left(a\varrho_0^{1/3}\right)^{2/3}. \tag{4.56}$$

Note that, for P a projection,

$$\begin{aligned}\|\gamma - P\|_1 &\leq \|(\gamma-1)P\|_1 + \|\gamma(1-P)\|_1 \\ &\leq \|P\|_2\|(\gamma-1)P\|_2 + \|\gamma^{1/2}\|_2\|\gamma(1-P)\|_2 \\ &\leq \|P\|_2\left[\operatorname{Tr}(1-\gamma)P\right]^{1/2} + \|\gamma^{1/2}\|_2\left[\operatorname{Tr}\gamma(1-P)\right]^{1/2}. \end{aligned} \tag{4.57}$$

Moreover,

$$\|\gamma^{1/2}\|_2^2 = \operatorname{Tr}\gamma \leq \operatorname{Tr}P + \operatorname{Tr}\gamma(1-P). \tag{4.58}$$

Note that $\operatorname{Tr}P_\mu \leq L^3(6\pi^2)^{-1}\mu^{3/2}$ (using Lemma 4). By combining the estimates (4.50), (4.51) and (4.56)–(4.58), with $P = P_\mu$ and $\gamma = \gamma_\uparrow^{X^\downarrow}$, we obtain that, for small $a^3\varrho_0$ and $\beta\varrho_0^{2/3} > (a^3\varrho_0)^{-1/9}$,

$$\frac{1}{L^3}\sum\!\!\!\!\!\!\int dX^\downarrow\, n(X^\downarrow)\, \left\|P_\mu - \gamma_\uparrow^{X^\downarrow}\right\|_1 \leq \text{const.}\left(a\varrho_0^{1/3}\right)^{1/6}. \tag{4.59}$$

This inequality supplements (4.38) in the case of large z.

It remains to estimate $\|P_\mu - \gamma_0\|_1 = \operatorname{Tr}P_\mu(1-\gamma_0) + \operatorname{Tr}\gamma_0(1-P_\mu)$. In the thermodynamic limit,

$$\begin{aligned}\lim_{L\to\infty}\frac{1}{L^3}\|P_\mu - \gamma_0\|_1 &= \frac{1}{(2\pi)^3}\int dp\left[\frac{\theta(\mu-p^2)}{1+ze^{-\beta p^2}} + \frac{\theta(p^2-\mu)}{1+z^{-1}e^{\beta p^2}}\right] \\ &\leq \frac{1}{(2\pi)^3}\int dp\left[\frac{\theta(\mu-p^2)}{ze^{-\beta p^2}} + \frac{\theta(p^2-\mu)}{z^{-1}e^{\beta p^2}}\right] \\ &\leq \frac{1}{6\pi^2}\frac{\mu^{1/2}}{\beta}\left(1+\frac{1}{2\beta\mu}\right), \end{aligned} \tag{4.60}$$

where the last inequality is derived in the same way as in (4.53)–(4.55). In case $\beta\varrho_0^{2/3} > (a^3\varrho_0)^{-1/9}$, as considered here, this last expression is actually bounded by $(a\varrho_0^{1/3})^{1/3}$, and therefore negligible compared with the error term on the right side of (4.59) for small $a^3\varrho_0$.

4.3.4 Summary of this subsection

To summarize, we have shown in this subsection that for a density matrix Γ satisfying $\mathcal{P}^L[\Gamma] \geq P_0^L(\beta,\mu) - Ca\varrho_0^2$ we have the *a priori* bound

$$\sum\!\!\!\!\!\!\int dX^\downarrow\, n(X^\downarrow)\,\left\|\gamma_{\text{per}} - \gamma_\uparrow^{X^\downarrow}\right\|_1 \leq C_\nu L^3\varrho_0\left(a\varrho_0^{1/3}\right)^{1/6-\nu} + o(L^3) \tag{4.61}$$

for $\nu > 0$, for some constant C_ν depending only on v (and C above), but not on z. Here, $\gamma_{\rm per}$ denotes the one-particle density matrix of a system of non-interacting fermions (at inverse temperature β and chemical potential μ) with periodic boundary conditions on the cube Λ_L.

As a side note, we remark that (4.61) implies, in particular, that the reduced one-particle density matrix of the dilute interacting system, $\gamma_\uparrow$, is close to the one for non-interacting particles. This, in turn, proves the inequality (1.8) in Corollary 1, with a worse error term than the one given in (1.8), however.

4.4 Putting Things Together

We now show how the estimates of the preceding subsections can be combined to prove the desired lower bound on the pressure, given in Theorem 1. Let h^χ be the one-particle operator given in (4.10). It follows from (4.11), (4.17) and (4.18) that, for any density matrix Γ,

$$
\begin{aligned}
-\tfrac{1}{2}L^3\mathcal{P}^L[\Gamma] \geq\ & \delta\, {\rm Tr}_{\mathcal{H}_1}[-\Delta\gamma_\uparrow] + {\rm Tr}_{\mathcal{H}_1}\left[(h^\chi-\mu)\,\gamma_\uparrow\right] - \frac{1}{\beta}\widetilde{S}[\gamma_\uparrow] \\
& +(1-\delta)(1-\varkappa)\,\rlap{\,/}\!\!\!\!\!\!\int\!\!\!\!\!\!\!\sum dX^\downarrow\, n(X^\downarrow)\,{\rm Tr}_{\mathcal{H}_1}\left[W_{X^\downarrow}\gamma_\uparrow^{X^\downarrow}\right]. \quad (4.62)
\end{aligned}
$$

Here, we used that Γ is symmetric with respect to exchange of the $\uparrow$ and $\downarrow$-particles, by assumption, which implies in particular that $\gamma_\downarrow = \gamma_\uparrow$. With the notation introduced in Lemma 7,

$$
{\rm Tr}_{\mathcal{H}_1}\left[(h^\chi-\mu)\,\gamma_\uparrow\right] - \frac{1}{\beta}\widetilde{S}[\gamma_\uparrow] \geq \frac{1}{\beta}f\big(\beta(h^\chi-\mu)\big). \quad (4.63)
$$

In the last term in (4.62), we use that

$$
{\rm Tr}_{\mathcal{H}_1}\left[W_{X^\downarrow}\gamma_\uparrow^{X^\downarrow}\right] \geq {\rm Tr}_{\mathcal{H}_1}\left[W_{X^\downarrow}\gamma_{\rm per}\right] - \|W_{X^\downarrow}\|_\infty \|\gamma_\uparrow^{X^\downarrow}-\gamma_{\rm per}\|_1. \quad (4.64)
$$

We have already estimated $\|W_{X^\downarrow}\|_\infty$ in (4.16), and this estimate is independent of $X^\downarrow$. Moreover, the $X^\downarrow$-average of $\|\gamma_\uparrow^{X^\downarrow}-\gamma_{\rm per}\|_1$ has been estimated in (4.61). Because of translation invariance, $\gamma_{\rm per}$ has a strictly constant density, given by $L^{-3}{\rm Tr}\,\gamma_{\rm per}$. Thus

$$
{\rm Tr}_{\mathcal{H}_1}\left[W_{X^\downarrow}\gamma_{\rm per}\right] = \frac{{\rm Tr}\,\gamma_{\rm per}}{L^3}\int_{[0,L]^3} dx\, W_{X^\downarrow}(x). \quad (4.65)
$$

We note that $L^{-3}{\rm Tr}\,\gamma_{\rm per} = \frac{1}{2}\varrho_0 + o(1)$ in the thermodynamic limit. To estimate the integral in (4.65), we write $W_{X^\downarrow} = W_+ - W_-$, where W_+

denotes the positive terms in (4.5) containing U, and $-W_-$ the negative ones containing w_R. For the negative part, we can use (4.13) to get the upper bound

$$\int_{[0,L]^3} dx\, W_-(x) \leq \text{const.}\, \frac{aR^2}{\varepsilon s^2} |X^\downarrow| \,. \tag{4.66}$$

Here, $|X^\downarrow| = M$ denotes the number of spin down particles. Note that

$$\sum\!\!\!\!\!\!\int dX^\downarrow\, n(X^\downarrow)\, |X^\downarrow| = \mathrm{Tr}\, \gamma_\downarrow \,. \tag{4.67}$$

This trace can be estimated using (4.61), which in particular implies that

$$\left| L^{-3} \mathrm{Tr}_{\mathcal{H}_1} \gamma_\downarrow - \tfrac{1}{2}\varrho_0 \right| \leq C_\nu L^3 \varrho_0 \left(a \varrho_0^{1/3} \right)^{1/6-\nu} + o(L^3) \,. \tag{4.68}$$

Moreover, using $\int U = 4\pi$,

$$\begin{aligned} \int_{[0,L]^3} dx\, W_+(x) &= \sum_{\{k\,:\, x_k^\downarrow \in \widetilde{X}_R^\downarrow\}} (1-\varepsilon) a \int_{[0,L]^3} dx\, U(x - x_k^\downarrow) \\ &\geq (1-\varepsilon) 4\pi a \left[\left| \widetilde{X}_R^\downarrow \right| - \text{const.}\, \frac{L^2}{R^2} \right] \end{aligned} \tag{4.69}$$

for any fixed $X^\downarrow$. Here, $|\widetilde{X}_R^\downarrow|$ denotes the number of elements in $\widetilde{X}_R^\downarrow$, i.e., the number of $x_k^\downarrow$'s in $X^\downarrow$ whose distance to the nearest neighbor among the $x_l^\downarrow$'s for $l \neq k$ is bigger than $2R$. The last term in square brackets bounds the number of $x_k^\downarrow$'s that are closer than a distance R to the boundary of the box. Since the distance between the $x_k^\downarrow$'s in $\widetilde{X}_R^\downarrow$ is bigger than $2R$, the number of such $x_k^\downarrow$'s close to the boundary is bounded by const. L^2/R^2.

We now need an estimate on $|\widetilde{X}_R^\downarrow|$. Note that

$$\left| \widetilde{X}_R^\downarrow \right| \geq \left| X^\downarrow \right| - (2R)^2 \sum_{k=1}^M \frac{1}{\delta_k^2} \,, \tag{4.70}$$

where δ_k denotes the distance of $x_k^\downarrow$ to its nearest neighbor in $X^\downarrow$. The last expression can be bounded from below using the operator inequality

$$\sum_{k=1}^M \frac{1}{\delta_k^2} \leq c \sum_{k=1}^M -\Delta_k^\downarrow \,, \tag{4.71}$$

which holds on the anti-symmetric tensor product $\bigwedge^M L^2(\mathbb{R}^3)$, and is proved in [6, Thm. 5]. Here, c is some positive constant satisfying $c \leq 48$. We thus have that

$$\sum\!\!\!\!\!\!\!\int dX^{\downarrow}\, n(X^{\downarrow})\,\big|\widetilde{X}_R^{\downarrow}\big| \geq \mathrm{Tr}_{\mathcal{H}_1}\left(1 + c(2R)^2\Delta\right)\gamma_{\downarrow}\,. \tag{4.72}$$

The negative last term involving the kinetic energy can be canceled by an appropriate choice of δ in (4.62).

By choosing $\delta = 2\pi ac\varrho_0(2R)^2$ and taking the thermodynamic limit $L \to \infty$ in (4.62), the above estimates imply that

$$\begin{aligned} P(\beta,\mu) \leq & -\limsup_{L\to\infty}\frac{2}{\beta L^3} f\big(\beta(h^\chi-\mu)\big) - 2\pi a\varrho_0^2\,(1-\delta-\varepsilon-\varkappa) \\ & + C_\nu a\varrho_0^2\left[\frac{R^2}{\varepsilon s^2} + \left(1+\frac{1}{\varrho_0}\max\left\{\frac{1}{R^3-R_0^3},\,\frac{1}{\varepsilon R s^2}\right\}\right)\left(a\varrho_0^{1/3}\right)^{1/6-\nu}\right]. \end{aligned} \tag{4.73}$$

It remains to estimate the first term on the right side of this expression. To this end, let $\Upsilon(p) = (1-\delta)p^2(1-(1-\varkappa)\chi(p)^2)$ (compare with (4.10)). We claim that

$$\liminf_{L\to\infty}\frac{1}{\beta L^3} f\big(\beta(h^\chi-\mu)\big) \geq \frac{-1}{(2\pi)^3\beta}\int_{\mathbb{R}^3} dp\,\ln\Big(1+z\exp\big(-\beta\Upsilon(p)\big)\Big)\,. \tag{4.74}$$

This can be seen using coherent states [2] as follows. Let u be a real function supported in a cube of side length ℓ, with $\int dx\,u(x)^2 = 1$, and let $\xi_{y,k}(x) = u(x-y)e^{ikx}$. Denoting by $|\xi_{y,k}\rangle\langle\xi_{y,k}|$ the projection onto $\xi_{y,k}$, we then have the resolution of identity $(2\pi)^{-3}\int dk\,dy\,|\xi_{y,k}\rangle\langle\xi_{y,k}| = 1$. Since $x \mapsto -x\ln x$ is concave for $0 \leq x \leq 1$, this implies that, for any fermionic one-particle density matrix γ,

$$\widetilde{S}[\gamma] \leq -(2\pi)^{-3}\int dk\,dy\,\Big[\varrho(y,k)\ln\varrho(y,k) + \big(1-\varrho(y,k)\big)\ln\big(1-\varrho(y,k)\big)\Big]\,, \tag{4.75}$$

where $\varrho(y,k) \equiv \langle\xi_{y,k}|\gamma|\xi_{y,k}\rangle$. Note that $0 \leq \varrho(y,k) \leq 1$, and that $\mathrm{Tr}\,\gamma = (2\pi)^{-3}\int dk\,dy\,\varrho(y,k)$. With $\widehat{\gamma}(k) = (2\pi)^{-3}\int dx\,dx'\,\gamma(x,x')\exp(ik(x'-x))$ denoting the Fourier transform of γ, we can write

$$\mathrm{Tr}\,h^\chi\gamma = \int dp\,\Upsilon(p)\widehat{\gamma}(p)\,. \tag{4.76}$$

Moreover, a simple calculation shows that

$$\int dk\,dy\,\Upsilon(k)\varrho(y,k) = (2\pi)^3\int dk\,dq\,\Upsilon(k+q)\widehat{\gamma}(k)|\widehat{u}(q)|^2\,. \tag{4.77}$$

Note that $\widehat{\gamma}(k) \geq 0$. In the case considered here, Υ has a bounded Hessian, i.e., $\partial_i \partial_j \Upsilon(k) \leq 2C$ as a matrix, for some constant C (depending only on the parameter s used in the definition (4.12) of χ). Therefore $\Upsilon(k+q) \leq \Upsilon(k) + q\nabla\Upsilon(k) + Cq^2$. Inserting this estimate into (4.77) and noting that $\int dq\, q|\widehat{u}(q)|^2 = 0$ since u is assumed to be real, we obtain

$$\mathrm{Tr}\,[h^\chi \gamma] \geq (2\pi)^{-3} \int dk\, dy\, \varrho(y,k) \left(\Upsilon(k) - C \int dx\, |\nabla u(x)|^2 \right) . \tag{4.78}$$

Now choose u such that $\int dx\, |\nabla u(x)|^2 \leq C' \ell^{-2}$ for some constant C' independent of ℓ. Then (4.75) and (4.78) imply that

$$\begin{aligned} &\mathrm{Tr}\,[(h^\chi - \mu)\gamma] - \frac{1}{\beta} \widetilde{S}[\gamma] \\ &\geq (2\pi)^{-3} \int dk\, dy\, \left(\Upsilon(k) - \mu - CC'\ell^{-2} \right) \varrho(y,k) \\ &\quad + \frac{1}{(2\pi)^3 \beta} \int dk\, dy\, \left[\varrho(y,k) \ln \varrho(y,k) + \big(1 - \varrho(y,k)\big) \ln \big(1 - \varrho(y,k)\big) \right] . \end{aligned} \tag{4.79}$$

Note that $\varrho(y,k) \neq 0$ only if y is an cube of side length $L+2\ell$. If we minimize the integrand for each fixed y (in this cube) and fixed k, we see that the right side of (4.79) is bounded from below by

$$-(L+2\ell)^3 \frac{1}{(2\pi)^3 \beta} \int dk\, \ln \left(1 + z e^{\beta CC'/\ell^2} e^{-\beta \Upsilon(k)} \right) . \tag{4.80}$$

Dividing by L^3, letting $L \to \infty$ and then $\ell \to \infty$ we arrive at (4.74).

It remains to estimate the integral on the right side of (4.74), and compare it with $-\frac{1}{2} P_0(\beta,\mu)$. We do this in two steps. First, note that

$$\begin{aligned} &\frac{2}{(2\pi)^3 \beta} \int dp\, \ln \left(1 + z e^{-\beta \Upsilon(p)} \right) - (1-\delta) P_0\big(\beta(1-\delta), \mu/(1-\delta)\big) \\ &= \frac{2}{(2\pi)^3 \beta} \int dp\, \ln \frac{1 + z e^{-\beta \Upsilon(p)}}{1 + z e^{-\beta(1-\delta)p^2}} . \end{aligned} \tag{4.81}$$

By the definition (4.12) of χ, $\Upsilon(p) = (1-\delta)p^2$ for $|p| \leq 1/s$. Hence the integrand in (4.81) is only non-zero for $|p| \geq 1/s$, in which case $\Upsilon(p) \geq (1-\delta)\varkappa p^2$. Hence (4.81) is bounded from above by

$$\begin{aligned} &\frac{2}{(2\pi)^3 \beta} \int_{|p| \geq 1/s} dp\, \ln \frac{1 + z e^{-\beta(1-\delta)\varkappa p^2}}{1 + z e^{-\beta(1-\delta)p^2}} \leq \frac{2z}{(2\pi)^3 \beta} \int_{|p| \geq 1/s} dp\, e^{-\beta(1-\delta)\varkappa p^2} \\ &\leq \frac{1}{\sqrt{2}\pi^2} \frac{1}{\beta^{5/2}} \frac{1}{(1-2\delta)\varkappa} e^{-\beta((1/2-\delta)\varkappa s^{-2} - \mu)} , \end{aligned} \tag{4.82}$$

where we estimated $|p| \leq (2\beta)^{-1/2}\exp(\frac{1}{2}\beta p^2)$ in the integrand in order to evaluate the last integral. Secondly, by simple scaling,

$$(1-\delta)P_0\big(\beta(1-\delta),\mu/(1-\delta)\big) = (1-\delta)^{-3/2}P_0(\beta,\mu)\,. \tag{4.83}$$

We thus arrive at the following estimate:

$$\begin{aligned} P(\beta,\mu) \;\leq\; & (1-\delta)^{-3/2}P_0(\beta,\mu) - 2\pi a\varrho_0^2\,(1-\delta-\varepsilon-\varkappa) \\ & + C_\nu a\varrho_0^2\left[\frac{R^2}{\varepsilon s^2} + \left(1+\frac{1}{\varrho_0}\max\left\{\frac{1}{R^3-R_0^3},\frac{1}{\varepsilon R s^2}\right\}\right)\big(a\varrho_0^{1/3}\big)^{1/6-\nu}\right] \\ & + \frac{1}{\sqrt{2}\pi^2}\frac{1}{\beta^{5/2}}\frac{1}{(1-2\delta)\varkappa}e^{-\beta((1/2-\delta)\varkappa s^{-2}-\mu)}\,, \end{aligned} \tag{4.84}$$

with δ given as above by $\delta = 2\pi ac\varrho_0(2R)^2$. It remains to choose s, R, ε and $\varkappa$. We take

$$R = \varrho_0^{-1/3}\big(a\varrho_0^{1/3}\big)^{1/22}\,,\ s = \varrho_0^{-1/3}\big(a\varrho_0^{1/3}\big)^{1/66}\,,\ \varepsilon = \big(a\varrho_0^{1/3}\big)^{1/33} \tag{4.85}$$

and

$$\varkappa = \big(a\varrho_0^{1/3}\big)^{1/33-\nu}\,. \tag{4.86}$$

Note that with this choice of parameters, $\delta = 8\pi c(a^3\varrho_0)^{12/33}$. Hence

$$\delta P_0(\beta,\mu) = \text{const.}\, a\varrho_0^2\big(a^3\varrho_0\big)^{1/33}\frac{P_0(\beta,\mu)}{\varrho_0(\beta,\mu)^{5/3}}, \tag{4.87}$$

and the last fraction is uniformly bounded for z bounded away from zero (as already argued in the lower bound after (3.47)). Moreover, since $\varkappa s^{-2} = \varrho_0^{2/3}(a^3\varrho_0)^{-\nu/3}$, we see by the same reasoning as in the lower bound in (3.45) that the last term in (4.84) is actually exponentially small in $a\varrho_0^{1/3}$, uniformly in z for bounded $1/z$. Inserting (4.85) and (4.86) into (4.84) above, we thus obtain

$$P(\beta,\mu) \leq P_0(\beta,\mu) - 2\pi a\varrho_0^2\left(1 - C_\nu(z)\big(a\varrho_0^{1/3}\big)^{1/33-\nu}\right) \tag{4.88}$$

for any $\nu > 0$, with $C_\nu(z)$ bounded for bounded $1/z$. This finishes the proof of the upper bound in Theorem 1.

5 Proof of Corollaries 1 and 2

In this final section, we show how to derive Corollaries 1 and 2 from Theorem 1. We start with proving Corollary 1. The essential ingredient is convexity of $P(\beta,\mu)$ in μ. It implies that

$$\varrho_-(\beta,\mu) \leq \varrho_+(\beta,\mu) \leq \frac{P(\beta,\mu+\delta)-P(\beta,\mu)}{\delta} \tag{5.1}$$

for any $\delta > 0$. Using (1.7) as well as the fact that $\varrho_0(\beta,\mu)$ is monotone increasing in μ, this yields

$$\begin{aligned} \varrho_+(\beta,\mu) \quad \leq \quad & \frac{P_0(\beta,\mu+\delta) - P_0(\beta,\mu)}{\delta} \\ & + \frac{1}{\delta} \varrho_0(\beta,\mu+\delta)^{5/3} C_\alpha\big(e^{\beta\mu}\big)\big(a\varrho_0(\beta,\mu+\delta)^{1/3}\big)^{1+\alpha} . \end{aligned} \tag{5.2}$$

Again by convexity, $P_0(\beta,\mu+\delta) - P_0(\beta,\mu) \leq \delta\varrho_0(\beta,\mu+\delta)$. We choose

$$\delta = \big(a\varrho_0(\beta,\mu)^{1/3}\big)^{(1+\alpha)/2} \max\{\mu,\, 1/\beta\} . \tag{5.3}$$

With this choice of δ, it is then not difficult to see that

$$\frac{\varrho_0(\beta,\mu+\delta)}{\varrho_0(\beta,\mu)} \leq 1 + \text{const.} \big(a\varrho_0^{1/3}\big)^{(1+\alpha)/2} \tag{5.4}$$

for some constant independent of μ and β. Using this estimate, (5.2) implies that

$$\varrho_+(\beta,\mu) \leq \varrho_0(\beta,\mu) \left(1 + \widehat{C}_\alpha(z)\big(a\varrho_0^{1/3}\big)^{(1+\alpha)/2}\right) \tag{5.5}$$

for some $\widehat{C}_\alpha(z)$ that is uniformly bounded for bounded $1/z$.

A lower bound on $\varrho_-(\beta,\mu)$ can be obtained similarly, using that, for $\delta > 0$,

$$\varrho_-(\beta,\mu) \geq \frac{P(\beta,\mu-\delta) - P(\beta,\mu)}{\delta} . \tag{5.6}$$

Proceeding along the same lines as in (5.1)–(5.5) above, this proves Corollary 1.

Next we prove Corollary 2. For $\varrho > 0$, let $f(\beta,\varrho) = \sup_\mu[\mu\varrho - P(\beta,\mu)]$ denote the free energy per unit volume. If the supremum is attained at some $\hat\mu$, then convexity of $P(\beta,\mu)$ in μ implies that

$$\varrho_-(\beta,\hat\mu) \leq \varrho \leq \varrho_+(\beta,\hat\mu) . \tag{5.7}$$

Let $f_0(\beta,\varrho) = \sup_\mu[\mu\varrho - P_0(\beta,\mu)]$ denote the free energy density for the ideal Fermi gas. The supremum is achieved at μ_0, determined by $\varrho_0(\beta,\mu_0) = \varrho$. Hence we immediately get the lower bound

$$f(\beta,\varrho) \geq \mu_0\varrho - P(\beta,\mu_0) \geq f_0(\beta,\varrho) + 2\pi a\varrho^2 - C_\alpha\big(e^{\beta\mu_0}\big)a\varrho^2\big(a\varrho^{1/3}\big)^\alpha , \tag{5.8}$$

where we used (1.7) to estimate $P(\beta,\mu_0)$ in terms of $P_0(\beta,\mu_0)$.

To get an upper bound on the free energy, we first make an *a priori* estimate to ensure that $\hat\mu$ is close to μ_0. Suppose that $\hat\mu < \mu_0$. Then, by

(5.7) and monotonicity of $\varrho_+(\beta,\mu)$ in μ, $\varrho = \varrho_0(\beta,\mu_0) \leq \varrho_+(\beta,\mu_0-\delta)$ for all $\delta \leq \mu_0 - \hat\mu$. Using (1.8), this implies that

$$\varrho_0(\beta,\mu_0) \leq \varrho_0(\beta,\mu_0-\delta)\left(1+K_\alpha(\beta,\mu_0-\delta)\right) \tag{5.9}$$

for all $\delta \leq \mu_0 - \hat\mu$, where we denoted

$$K_\alpha(\beta,\mu) = \widehat{C}_\alpha(e^{\beta\mu})\left(a\varrho_0(\beta,\mu)^{1/3}\right)^{(1+\alpha)/2}. \tag{5.10}$$

Ineq. (5.9) then implies that

$$\delta \leq \text{const.}\left(a\varrho^{1/3}\right)^{(1+\alpha)/2} \max\{\mu_0,\, 1/\beta\} \tag{5.11}$$

for some constant independent of ϱ and β (compare with (5.3)). Denoting the right side of (5.11) by $\bar\delta$, we therefore see that $\hat\mu \geq \mu_0 - \bar\delta$.

The same method works in the case when $\hat\mu > \mu_0$. One uses that $\varrho_0(\beta,\mu_0) \geq \varrho_-(\beta,\mu_0+\delta)$ for all $\delta \leq \hat\mu - \mu_0$. Proceeding along the same lines, this implies that $\hat\mu \leq \mu_0 + \bar\delta$. In particular,

$$f(\beta,\varrho) = \sup_{|\mu-\mu_0|\leq\bar\delta}\left[\mu\varrho - P(\beta,\mu)\right]. \tag{5.12}$$

Using (1.7) and (1.8), it is not difficult to see that

$$P(\beta,\mu) \geq P_0(\beta,\mu) - 2\pi a\varrho_0(\beta,\mu_0)^2\left(1+\widetilde{C}_\alpha\left(e^{\beta\mu_0}\right)\left(a\varrho_0(\beta,\mu)^{1/3}\right)^\alpha\right) \tag{5.13}$$

if $|\mu-\mu_0| \leq \bar\delta$, for some $\widetilde{C}_\alpha(z)$ that is uniformly bounded for bounded $1/z$. Inserting the bound (5.13) into (5.12) proves the desired upper bound on $f(\beta,\varrho)$.

Note that $e^{\beta\mu_0}$ is bounded away from zero for bounded $1/(\beta\varrho^{2/3})$. Hence (5.13) and (5.8) imply the statement in Corollary 2.

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